

Ecology Quick Chemical Assessment Tool 1.2 Methodology

Beta-Max Version

Alex Stone, Sc. D.

Washington State Department of Ecology

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Disclaimer:

Although the Quick Chemical Assessment Tool is based upon methodology developed by the US EPA Design for the Environment Program subsequently adapted by Clean Production Action as the GreenScreen™, this should not be taken as an endorsement of the Quick Chemical Assessment Tool by either organization. The Quick Chemical Assessment Tool remains the sole product of the Washington State Department of Ecology who is responsible for its contents and implementation.

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1. Introduction

As concern has increased about the widespread use of toxic chemicals in products and the overall effect these chemicals have upon human health and the environment, issues have arisen around the replacement of these chemicals of concern with safer alternatives. Previously, there have been several instances where chemicals of concern have been replaced with chemicals that have shown to pose an equal or greater hazard than the original. This process is called ‘regrettable substitution’ and several cases have been widely documented.

One well-documented example is the replacement of chlorinated solvents in the auto repair industry with hexane. (CDC, 2001) In response to increasing regulation of methylene chloride and other halogenated solvents, several manufacturers switched from chlorinated solvents to hexane for products such as brake cleaners. This substitution was done without determining if any hazards were associated with the substitute. Hexane was known to cause nerve damage as early as 1964 (Yamada, 1964). A few years after the substitution, workers in auto repair shops in California began to report health concerns eventually tied to hexane. (Berkeley, 2010) Examples such as this have emphasized the need for methodologies to compare chemicals of concern with potential substitutes to guarantee that products are both toxic free and safe for use.

EPA took the early lead in this field and established the Design for the Environment (DfE) Program in the late 1990’s. DfE pioneered work in the field of alternative assessments by developing a series of hazard criteria used to compare chemicals of concern with potential substitutes. These criteria have undergone revision and DfE released an update of the hazard criteria in 2011. (DfE, 2011) These criteria form the basis of an alternative assessment methodology DfE continues to use in its alternative assessment program.

In addition, DfE established a voluntary program with several manufacturers of consumer products and, by implementing these criteria, created the DfE labeling program. Each ingredient in those products earning the label has undergone review by DfE. Each ingredient in the formulation has the lowest possible impact upon human health and the environment in their functional class while maintaining product function at a reasonable cost. Since the inception of the labeling program, more than 2,500 products carry the DfE label. (DfE, 2012)

Subsequently, other organizations have taken the DfE hazard criteria and alternative assessment process and adapted them for use by a wider audience. A non-profit group, Clean Production Action (CPA) was one of the earliest adopters. CPA adapted the DfE criteria and methodology and created the GreenScreen™ (GS™), an alternative assessment tool that emphasizes transparency when conducting an alternative assessment program. (CPA, 2012) CPA tested out the new GS™ methodology by conducting an alternative assessment of the flame retardant, decabromodiphenyl ether. (CPA, 2007) Since that time several other companies and organizations, including the Washington State Department of Ecology (Ecology), have adopted the GS™ as a tool for conducting alternative assessment. Ecology used the GS™ during its assessment of decabromodiphenyl ether use in electronic enclosures and residential upholstered furniture. (Ecology, 2009) Other organizations also using the GS™ include the Green Chemistry and Commerce Council (GC³, 2012) and Hewlett-Packard (Lavoie, 2010).

During this process, however, it was recognized that, although these tools are excellent and provide the highest degree of certainty against a regrettable substitution, they also require a high degree of technical expertise and resource allocation to do correctly. These limitations make it very difficult for small and medium businesses with limited resources and expertise to conduct any degree of alternative assessment. It is for this reason that Ecology has begun the development of the Quick Chemical Assessment Tool (QCAT).

The QCAT is based on the GS™ although it neither is as comprehensive nor as detailed in its evaluation. The objective, however, was to provide a simpler tool that smaller businesses can implement and at least have a small degree of assurance they are not replacing a toxic chemical with another chemical already identified as having hazard concerns. Because the QCAT is less comprehensive than the GS™, users should realize that there is a greater risk of making a regrettable substitution than if a full GS™ was conducted. Given that limitation, the QCAT does allow small and medium businesses to become familiar with the alternative assessment process. It also enables them to identify chemicals that are clearly poor substitutes and potentially to dedicate limit resources to do a more comprehensive alternative assessment on those alternatives that look most promising. However, since the QCAT is based upon the GS™, we will first provide an overview of the GS™, followed by a detailed description of the QCAT including how the QCAT is similar and different from the GS™, and how to use the QCAT.

1. GreenScreen™ Background

The primary objective of the GS™ is to evaluate chemicals and their potential degradation products against a wide range of toxicity, environmental fate and physical/chemical endpoints to determine safer chemical alternatives to chemicals of concern. Chemicals receive a Benchmark score based upon the combination of the hazard assessments of 19 endpoints (18 required and 1 optional):

Hazard Criteria

Human Health Effects

Group I

- Carcinogenicity (C)
- Mutagenicity & Genotoxicity (M)
- Reproductive toxicity (R)
- Developmental toxicity (including Developmental Neurotoxicity) (D)
- Endocrine Activity (E)

Group II

- Acute Mammalian Toxicity (AT)
- Systemic Toxicity & Organ Effects (including Immunotoxicity) (ST)
- Neurotoxicity (N)

- Sensitization: Skin (SnS)
- Sensitization: Respiratory (SnR)
- Irritation/Corrosivity: Skin (IrS)
- Irritation/Corrosivity: Eyes (IrE)

Environmental Health

- Acute Aquatic Toxicity (AA)
- Chronic Aquatic Toxicity (CA)
- Other Ecotoxicity Studies, when available (optional except for BM 4) (Eo)

Environmental Fate

- Persistence (P)
- Bioaccumulation (B)

Physical/Chemical Properties

- Reactivity (R)
- Flammability (F)

The GS™ requires a high level of technical expertise as specialists in toxicology, chemistry, computer modeling and other scientific areas are needed to generate data, evaluate sources, review technical information and assign benchmark scores to the chemicals which have undergone the screening process. This is particularly true when information from peer reviewed journal articles and computer modeling are used to fill in data for all hazard endpoints.

The GS™ also requires a commitment of time and resources and, therefore, is costly to implement. In order to address some of these concerns, the current GS™ coordinates with other regulatory requirements (GHS¹, REACH², etc.) and uses authoritative lists to provide established criteria for those chemicals for which toxicity concerns have already been identified. This enables different individuals and organizations to implement the GS™ and reach similar conclusions, i.e. consistent results from different individuals and/or organizations performing an assessment on the same chemical using ‘professional judgment’. If data is not found using easily accessible sources that require little interpretation by the user, more technical sources requiring a higher level of interpretation are used to provide a complete data set for evaluation.

As with many aspects of the GS™, the level of expertise required to evaluate data and determine whether or not it can be used increases as the data sources become more technical and detailed. It may also be necessary to call upon individuals with specialized degrees such as toxicologists,

¹ GHS stands for the United Nation’s Global Harmonization System. The GHS requires labeling of chemicals for a wide range of hazard criteria.

² REACH stands for the European Union’s Registration Evaluation and Authorisation of CHemicals legislation. REACH establishes data requirements for any chemical manufactured or imported into the European Union.

chemists, (Q)SAR³ specialists, etc. to provide a professional evaluation of specific sources. For example, Ecology commissioned SRC (formerly Syracuse Research Corporation) to collect data and generate (Q)SAR data for hazard endpoints and other toxicity data for Ecology's chemical action plan (CAP) on the polybrominated diphenyl ether (PBDE) family of flame-retardants. (Ecology, 2006) The data was subsequently used for the deca-BDE alternative assessment.

Based upon this detailed scientific evaluation, the GSTM provides the highest degree of certainty that the assessment is valid and comprehensive. Because of the evolving nature of science including toxicology, some degree of uncertainty will always exist for any hazard evaluation methodology including the GSTM. Therefore, it is very important that all chemicals and products should be subjected to periodic review to evaluate the impact of improvements in data and scientific understanding upon the classification of chemicals and the final benchmark assigned from a particular evaluation.

The GSTM places chemicals along a continuum of concern and assigns a chemical one of four possible benchmarks as described in Table 1:

Table 1: Benchmarks from the GSTM assessment process

| | | |
|--------------------|-----------------------------------|---------------------------------|
| Benchmark 4 | Few concerns, i.e. safer chemical | Preferable |
| Benchmark 3 | Slight concern | Improvement possible |
| Benchmark 2 | Moderate concern | Use but search for safer |
| Benchmark 1 | High concern | Avoid |

The result of this benchmarking process enables chemicals to be identified as safer alternatives to existing chemicals of concern and emphasizes the removal of chemicals of high concern (Benchmark 1) from the manufacturing stream and product design. These chemicals are typically one or more of the following:

1. Persistent, bioaccumulative and toxic (PBT).
2. Very persistent and very bioaccumulative (vPvB).
3. Identified as possessing a high level of hazard for a priority human health effect such as CMR (carcinogenicity, mutagenicity or development toxicity), etc.

Based upon this analysis, it is possible to identify safer alternatives to chemicals of concern in a clear and reproducible manner.

2. Quick Chemical Assessment Tool (QCAT)

³ (Q)SAR stands for Quality Structure Activity Relationships. (Q)SARs are computer modeling results that predict the toxicity of chemicals based upon structural similarities with chemicals possessing known toxicity concerns.

Because of the high level of technical and resource commitments required by the GS™, a simpler alternative called the Quick Chemical Assessment Tool (QCAT) has been developed by the Ecology). The primary goal of the QCAT is to assign an appropriate grade for a chemical using both 1) a subset of high priority hazard endpoints identified in the GS™ and 2) fewer data sources. This information can be used to provide an approximation of the concerns associated with chemicals based upon the limited data used in the evaluation process.

The results of a QCAT assessment are therefore based upon fewer data and there is an increased chance of an incomplete assessment that could result in a chemical with concerns being missed during this evaluation process. In other words, the uncertainty associated with the QCAT assessment is greater than with a GS™ review. To complete a GS™ assessment, data must be obtained and evaluated for each of the 19 hazard endpoints. However, QCAT assessments examine 9 hazard endpoints – priority human health effects (6 endpoints), persistence, bioaccumulation and acute aquatic toxicity – that drive identifying a level of concern for each chemical being evaluated.

One benefit of the QCAT, however, is that it provides a quick and easy method to identify chemicals that are equally or more toxic than the chemical being reviewed. Therefore, limited resources can quickly identify chemicals that are not viable alternatives to the chemical being assessed. Because of the reduced amount of information assessed, a QCAT review is not as good at identifying truly preferable alternatives to the chemical undergoing assessment. If resources are limited, however, QCAT can be used to quickly eliminate non-viable alternatives and remaining resources can be used to investigate the chemicals that pass a QCAT review.

The QCAT places chemicals along a continuum of concern and assigns a chemical one of four possible grades as shown in Table 2:

Table 2: Grade levels from the QCAT assessment process

| | | |
|----------------|-----------------------------------|---------------------------------|
| Grade A | Few concerns, i.e. safer chemical | Preferable |
| Grade B | Slight concern | Improvement possible |
| Grade C | Moderate concern | Use but search for safer |
| Grade F | High concern | Avoid |

The grading system for the QCAT is substantively different from the benchmarking system used for the GS™. The differences emphasizes that the QCAT is not as comprehensive as the GS™ and that the risk of assigning an incorrect grade is greater. However, the QCAT will clearly identify Grade F (red) chemicals that should be targeted for removal from the manufacturing stream.

A secondary goal of the QCAT is to identify and prioritize additional research required to conduct a GSTM assessment. The QCAT can quickly identify chemicals of concern and could be used to prioritize chemicals at a particular manufacturing facility for a more detailed review. This would separate these chemicals from others that do not require immediate attention.

There are several advantages to evaluating chemicals using the QCAT. The QCAT focuses on important hazard endpoints, lowers data requirements and provides a significant amount of information with relatively low investment of resources in comparison with a GSTM assessment. There are disadvantages of performing a QCAT rather than a GSTM assessment. With a focus on a few focused hazard endpoints, not all hazard endpoints are evaluated. It is possible that an endpoint of concern could be overlooked, either because the screening assessments did not highlight the endpoint or because new data have been developed that have not yet been reviewed by key information sources.

For example, new carcinogenicity data may have been generated on a chemical that has not yet been reviewed by International Agency for Research on Cancer (IARC) or the US EPA. A GSTM would include more recent information that would be missed by the QCAT. The QCAT also provides less breadth and depth in evaluating data to determine levels of concern for hazard endpoints. Thus, performing a GSTM assessment using a comprehensive weight of evidence approach with all available data may result in a different level of concern being assigned than the level of concern assigned by a QCAT assessment of the same chemical for some endpoints.

Lastly, as more hazard information becomes available via the implementation of such regulation as the European Union's REACH and implementation of the Global Harmonization System, data may become available that was not used in the QCAT evaluation. This new data may alter the conclusions reached; therefore, it is important that users revisit the QCAT evaluation periodically. Even with its limitations, the QCAT is a useful and efficient initial step in assessing chemical alternatives.

Identify Chemical Abstract Services (CAS) Number(s)

Analysis of chemicals using the QCAT is based upon the Chemical Abstracts Service's (CAS) number. CAS numbers are assigned by the American Chemical Society and are unique to a specific chemical. Therefore, although a chemical may have many different common or product names, it will typically have only a single CAS number. Occasional errors do occur and a chemical may have more than one CAS identifier; however, those instances are rare and should have minimal impact upon the QCAT assessment process.

When a chemical is being evaluated, it simplifies the process if a CAS number is used to reduce confusion caused by varying and numerous names often associated with a particular chemical.

CAS numbers may be readily available from the chemical supplier. If a CAS number is not readily available, it may be obtained from authoritative sources such as the Hazardous Substances Database (HSDB), the Registry of Toxic Effects of Chemical Substances (RTECS) or other authoritative sources. Information on these three sources is available in Appendix 2. If unsuccessful, the CAS number may be obtained from an Internet search. Without a CAS, a specific chemical cannot undergo the assessment.

QCAT Hazard Endpoints

For the purpose of the QCAT, the hazard endpoints in Table 3 have been selected for evaluation. These hazard endpoints have been selected as those which pose the greatest threat to sensitive populations such as children and provide a good indication of the risks posed by chemicals. In addition, with the exception of endocrine activity, the hazard endpoints selected for evaluation in the QCAT are among the most widely studied and are most likely to be reported in the sources selected for the QCAT assessment. Although authoritative data on endocrine active compounds are scarce, current information on the potentially widespread impact endocrine active substances are having upon human health and the environment warrant inclusion. The selected hazard endpoints including endocrine activity also coincide with Ecology priorities as demonstrated in legislation and initiatives such as the Children's Safe Product Act, the Puget Sound Initiative and the Reducing Toxic Threats program.

Table 3: QCAT Hazard Endpoints Compared with the GS™

| | QCAT | GS™ |
|--|------|-----|
| Human Health: | | |
| Tier I | | |
| • Carcinogenicity (C) | X | X |
| • Mutagenicity & Genotoxicity (M) | X | X |
| • Reproductive toxicity (R) | X | X |
| • Developmental toxicity (incl. developmental neurotoxicity) (D) | X | X |
| • Endocrine activity (E) | X | X |
| Tier II | | |
| • Acute Mammalian Toxicity (AT) | X | X |
| • Systemic & organ effects toxicity incl. Immunotoxicity (ST) | | X |
| • Neurotoxicity (N) | | X |
| • Sensitization: Skin (SnS) | | X |
| • Sensitization: Respiratory (SnR) | | X |
| • Irritation & Corrosivity: Skin (IrS) | | X |
| • Irritation & Corrosivity: Eye (IrE) | | X |
| Ecological: | | |

| | | |
|--|----------------|---|
| • Acute Aquatic Toxicity (AA) | X | X |
| • Chronic Aquatic Toxicity (CA) | | X |
| • Other Ecotoxicity Studies, when available (optional except for Benchmark 4) (Eo) | | X |
| Environmental: | | |
| • Persistence (P) | X ⁴ | X |
| • Bioaccumulation (B) | X | X |
| Physical: | | |
| ▪ Reactivity (R) | | X |
| ▪ Flammability (F) | | X |

One further advantage to the fewer number of hazard endpoints included in the QCAT is that the difference clearly distinguishes results for a QCAT assessment from results for a GSTM assessment. By including a wider range of hazard endpoints and requiring more detailed evaluation of the hazards involved, the GSTM provides a greater degree of certainty concerning the hazards associated with each chemical. By subjecting chemicals to the QCAT, there is the potential to identify chemicals requiring further review.

It is important to reiterate at this point that by evaluating fewer hazard endpoints, there is a greater risk that chemicals of concern may be missed by the QCAT. However this increased risk is compensated for by the improved ability to implement the QCAT and the reduced implementation costs. The QCAT also makes it easier for users to begin to understand the safer chemical alternative process and provides concerned and interested parties a chance to start providing safer products.

It is also important to note that the QCAT only looks at hazard-related criteria. Most alternative assessments must consider other factors such as process engineering, availability, existing usage, cost, energy balance, exposure, etc. Therefore, although the QCAT is an important component of an alternatives assessment, other factors must also be considered before a safer alternative can be identified.

QCAT Data Sources

Use of authoritative lists and summarized data sources leverages expert judgment and provides a reliable initial assessment of the hazards that should be considered in evaluating a chemical. Appendix 1 provides authoritative lists to be used in Step I of the evaluation.

⁴ Not needed if the assessment is done solely for inorganic compounds as all inorganics are assumed to be persistent. Clean Production Action is creating specialized rules for dealing with inorganic compounds and these rules will be incorporated into QCAT once they have been finalized and released for use with the next GSTM update.

Data sources used to complete the QCAT for the 9 hazard endpoints are selected in two steps. These steps, itemized in Table 4, are not unique to the QCAT. They are informed by the data requirements in the GS™ and those used by EPA in its Design for the Environment (DfE) program.

There is an increasing level of technical expertise necessary to review the information at each Step. For example, Step I sources require little technical review or expertise and only a basic understanding of the hazard endpoints. The user simply determines whether or not a chemical appears in the authoritative sources that have been reviewed and approved by recognized experts in each field. Step II requires sufficient technical expertise to evaluate the information in the sources and reach a defensible conclusion about the applicability of the data to the QCAT. QCAT includes instruction on how to interpret and find data from Step II sources, which will reduce the need for technical expertise. Additional steps in a GS™ evaluation (not included) require experts knowledgeable and experienced in evaluating specific hazard endpoints. These advanced steps will not be used during a QCAT evaluation as the technical expertise needed to review scientific journal articles and assess studies for completeness and technical accuracy is outside the scope of this method.

Table 4: Two Steps of data collection for the QCAT

| Data sources |
|--|
| Step I: Authoritative Sources: (toxicity characteristics lists, databases, etc. generated by internationally recognized authoritative bodies or appropriate government agencies.) |
| Step II: Other Data Sources Estimated Data: PBT Profiler, other non-sophisticated modeling results Measured data: Specific information from publicly available risk assessments and databases such as RTECS, ECOTOX, HSDB, etc. |

Chemicals identified as a concern in Step I will not be evaluated further. Presence in any Step I list is deemed authoritative. Only those chemicals that do not appear in Step I sources will be subjected to further, Step II review. Presence on any single Step I source is sufficient for assigning a ranking to the chemical being evaluated. It is recommended for Step II sources that two individual sources agree on the ranking; however, if only one set of data is available from Step II sources, it is sufficient for assigning a rank. The final QCAT report should document that only one Step II data source was located and further review might be warranted.

For the purposes of the QCAT, the databases in Steps I and II will be searched for applicable toxicity data pertinent to assigning a ranking. No attempt, however, will be made to review the sources identified in the database as it is assumed these sources have already undergone peer review by experts before being referenced in the databases. Therefore the databases are assumed

authoritative for the purposes of the QCAT and further review is not needed. For example, the HSDB often contains information on toxicity values that are applicable to assigning a grade for a chemical. No attempt, however, will be made to evaluate the sources of these values as such a review would require a higher degree of technical expertise than is expected for implementation of the QCAT.

One should remember that the QCAT hazard endpoints are not the only information that needs to be evaluated as part of a safer chemical alternative assessment. One must evaluate whether the alternative can be used in the manufacturing process, whether it is generally available, if the cost differential is reasonable, etc. However, a QCAT evaluation is an important step in evaluating chemicals, which undergo the subsequent evaluation process. Chemicals that fail the QCAT process are not viable alternatives and need no further evaluation.

Several organizations have compiled lists of chemicals of concern using these authoritative sources and these databases include many of the sources used in a Step I evaluation. Users, therefore, may not need to compile a list of their own or need to decipher the information on all the individual sites but may defer to some of these compilations. The University of California-Berkeley has developed such a resource. Plum (Public Library of Materials) ‘... is a free, open-access resource for finding authoritative information about the known hazards of thousands of chemicals.’⁵ Plum allows users to search on a chemical and identifies data from authoritative bodies that have listed the chemical as a chemical of concern. One major advantage of this site is that it pulls together a wide range of current information and makes it freely available to all interested parties.

Ecology has developed a list of High Priority Chemicals as part of its implementation of the Children’s Safe Product Act that compiles these chemicals into one specific source.⁶ The list will be updated to add or remove chemicals. The State of Maine has also generated a similar list of chemicals of concern based upon many of the same sources, and their list is publicly available.⁷ Minnesota also has a list.⁸ Several other lists exist, so a user may wish to review the different compilations and decide if any would assist in the evaluation process. The Interstate Chemicals Clearinghouse (IC2) has compiled these lists into a single source. A user can search

⁵Plum, Public Library of Materials, University of California-Berkeley at <http://plm.berkeley.edu/>, accessed 1/5/2012.

⁶ For more information on this list information see Stone and Delistraty (http://www.sciencedirect.com/science?_ob=ArticleURL&_udi=B6V9G-4Y5H5XP-1&_user=10&_rdoc=1&_fmt=&_orig=search&_sort=d&_docanchor=&view=c&_acct=C000050221&_version=1&_urlVersion=0&_userid=10&md5=6cbd6a426cb849743c8d27f7da883874) or the Washington’s CSPA website (<http://www.ecy.wa.gov/programs/swfa/rules/ruleChildPilotPhase.html>), accessed 1/2012.

⁷ Maine’s list is available at: <http://www.maine.gov/dep/safechem/highconcern/index.html>, accessed 1/2012.

⁸ Minnesota’s list is available at: <http://www.health.state.mn.us/divs/eh/hazardous/topics/toxfreekids/highconcern.html#list>

the IC2 database and find out information on if a chemical was identified by a specific state and what toxicity criteria caused it to be placed on the state list.⁹

Lastly, pay sites are being or have been developed that provide similar information. Healthy Building Network has developed Pharos, a database that contains some of the information found in Step I sources. Pharos creators define it as ‘...a partnership, pairing those who use building materials with those who study the products’ impacts on health and the environment.’¹⁰ Pharos, like the GSTM also benchmarks chemicals into different categories so care should be taken not to confuse these with the GSTM benchmarks¹¹. The raw data in Pharos is only available to those who pay a nominal yearly fee, currently at \$180 per year. Other pay options are also available either on a monthly basis or for multiple users from a single organization.

An automated version of the authoritative lists used in the GSTM, the GreenScreen LiTeTM (GSLTM), is currently under development and will be another source of information. The GSLTM tool is being developed through a partnership between Clean Production Action, the developers of the GSTM methodology, and The WerCS, a a hazard communication authoring software platform and regulatory content provider¹². The GSLTM compares chemicals against data in authoritative lists for all 18 hazard endpoints and identifies any chemicals for which concerns have been identified. Costs for the GSLTM tool have not yet been determined, but it is likely the service will be available as part of The WerCS standard services for which a fee is charged on a monthly basis. Once this service is developed, it may provide a viable alternative to conducting Step I evaluation of lists included in QCAT.

QCAT users can save appreciable time by checking free websites like Plum and the IC2 database or pay sites like Pharos or the GSLTM (if they have memberships) first before proceeding to other sources of information. Caution should be taken, however, as sites like these may not be current or include recent additions or deletions from the authoritative sources. As an initial point for information, they can prove very useful to the QCAT user.

QCAT Grading Processes

The QCAT grading process is based upon similar processes established for the GSTM. The only difference between the QCAT and GSTM processes is the amount of information used to assign a score. As the GSTM uses more hazard endpoints than the QCAT, the GSTM data gap and benchmarking processes are more involved. For the purposes of the QCAT, the scoring process

⁹ The IC2 database is available at: <http://www.newmoa.org/prevention/ic2/projects/resource/>, accessed 1/2012.

¹⁰ Information on Pharos is available at: <http://www.pharosproject.net/about/index/>, accessed 1/2012.

¹¹ Information on Pharos content and benchmarking available at: <http://staging.pharosproject.net/material/>, accessed 1/2012.

¹² Information on The WerCS is available at: <http://www.thewerCS.com/products-and-services/greenwerCS>, accessed 1/2012.

is simplified. This, however, is the major difference between the two methods. Any future changes to the GS™ data gap and benchmarking processes will be evaluated and, if appropriate, reflected in changes to similar QCAT processes.

The first step in the grading process is to assign a degree of concern for all the data obtained from Step I and II sources. The ranking process is based upon the methodology originated by EPA's DfE Program. (DfE, 2011) The data found is compared to the ranking criteria established by DfE and assigned one of five ranking ranging from very high (royal purple), high (red), moderate (yellow), low (green) and very low (blue). The color coding provides a very visual representation of the level of concern associated with each hazard criteria for the chemical under consideration.

The ranking results are visually displayed in Table 5:

Table 5: Example of QCAT Reporting Table

| Human - Group 1 | | | | | Human - Group 2 | | | | | | | Env. Health | | | Fate | | Physical | |
|-----------------|---|---|---|---|-----------------|----|---|-----|-----|-----|-----|-------------|----|----|------|---|----------|---|
| C | M | R | D | E | AT | ST | N | SnS | SnR | Irs | IrE | AA | CA | Eo | P | B | Ex | F |
| - | - | - | - | - | - | ? | ? | ? | ? | ? | ? | - | ? | ? | - | - | ? | ? |

Each box is highlighted with the correct color to show the level of concern. The same table is used to report QCAT and GS™ results and includes all of the criteria including those not included in the QCAT assessment. A question mark (?) is used to represent information not included in the QCAT assessment and is a representation of the increased risk involved with conducting a more restricted analysis like QCAT as opposed to a more comprehensive review like GS™.

Once the level of concern has been identified using all existing data, the next step is to assign a grade to each chemical. QCAT grading is based upon the GS™ process and it will be updated with any future changes to the GSTM process. A grade is based upon comparing the levels of concern for the 9 QCAT hazard criteria using the following decision logic:

| | |
|----------------|---|
| Grade A | <ul style="list-style-type: none"> Low P + Low T (AA, AT and all HH endpoints). |
| Grade B | <ul style="list-style-type: none"> Moderate P; or Moderate B; or Moderate AA; or Moderate AT or one or more HH endpoints. |
| | <ul style="list-style-type: none"> Moderate P + Moderate B + Moderate T (AA, AT, or any HH endpoint); or |

| | |
|----------------|---|
| Grade C | <ul style="list-style-type: none"> • High P & High B; or • High P + Moderate T (AA, AT, or any HH endpoint); or • High B + Moderate T (AA, AT, or any HH endpoint); or • Very High T (AA or AT) or High T (any HH endpoint). |
| Grade F | <ul style="list-style-type: none"> • PBT = High P + High B + [Very High T (AA or AT) or High T (HH)]; or • vPvB = very High P + very High B; or • vPT = very High P + [very High T (AA or AT) or High T (HH)]; or • vBT = very High B + [very High T (AA or AT) or High T (HH)]; or • High T (HH). |

Legend:

| | |
|---------------------------------------|---|
| AA = Acute Aquatic Toxicity | P = Persistence |
| AT = Acute Mammalian Toxicity | PBT = Persistent, Bioaccumulative & Toxic |
| B = Bioaccumulation | R = Reproductive toxicity |
| C = Carcinogenicity | T = Toxic |
| D = Developmental Toxicity | vBT = very Bioaccumulative & Toxic |
| E = Endocrine Activity | vPT = very Persistent & Toxic |
| HH = Human Health (C, M/G, R, D & EA) | vPvB = very Persistent & very Bioaccumulative |
| M = Mutagenicity/Genotoxicity | PBT = Persistent, Bioaccumulative & Toxic |

The grading process begins by evaluating the data available against the Grade F criteria. If none of the Grade F criteria are met, the available data is compared against the Grade C criteria and so forth until a grade is determined.

QCAT Data Gap and Grading Processes

Once an initial grade has been assigned, the chemical must be subjected to a data gap analysis. As with the grading process itself, the data gap analysis is similar to the process established for the GS™. It has been somewhat simplified to compensate for the fewer hazard criteria although the overall logic process is the similar. The data gap process reviews the data gaps found in the chemical ranking table for a specific chemical and, if necessary, reduces the grade's final grade based upon the number and relative importance of the data gaps. The following is the QCAT data gap analysis process:

Grade F: Any chemical that qualifies for a Grade F will not undergo a data gap analysis. Grade F is the lowest possible grade to which any chemical can be assigned. Therefore any data gaps would only reinforce the assignment of a Grade F and is unnecessary. If your chemical has attained a Grade F based upon existing data, continue with the review of other alternatives.

Note: The QCAT user is cautioned in placing confidence in any grade assigned to a chemical above the Grade F. Because the QCAT uses fewer criteria and less data, the risk of incorrectly

assigning any chemical a grade above F increases substantially. The QCAT user, however, may wish to proceed and use the other grades as a further prioritization tool to winnow down potential alternatives. Those chemicals that receive the best QCAT grade may be subjected to a more complete GS™ analysis to increase confidence in the chemical's actual ability to function as a safer alternative to the chemical of concern.

Grade C: If a chemical has been assigned a Grade C based upon existing data, it is necessary to see if any data gaps could potentially adversely affect this grading. Based upon what data is missing, the following evaluations must be made:

- Does the chemical ranking table contain a data gap for any of the following hazard endpoints: Mutagenicity/Genotoxicity, Acute Mammalian Toxicity, Persistence, Bioaccumulation or Acute Aquatic Toxicity?
- Does the chemical ranking table contain more than two data gaps?
- Does the chemical ranking table contain two data gaps and are those two anything other than Endocrine Activity and either Carcinogenicity, Reproductive Toxicity or Developmental Toxicity?

If the answer is 'yes' to any of the above questions, the chemical is assigned a Grade F_{dg}. The 'dg' indicates the chemical is assigned a Grade F based upon serious data gaps. This communicates that, although the chemical is provisionally assigned a Grade F, its grading can be revisited once information is available to fill in the missing data.

Grade B: If a chemical has been assigned a Grade B based upon existing data, it is necessary to see if any data gaps could potentially adversely affect this grading. Based upon what data is missing, the following evaluation must be made:

- Does the chemical ranking table contain two or more data gaps for the following hazard endpoints: Carcinogenicity, Reproductive Toxicity, Developmental Toxicity, Mutagenicity/Genotoxicity, Endocrine Activity or Acute Mammalian Toxicity?
- Does the chemical ranking table have a data gap for only one hazard endpoint and is that endpoint anything other than Endocrine Activity?
- Does the chemical ranking table contain a data gap for any of the following criteria: Persistence, Bioaccumulation or Acute Aquatic Toxicity?

If the answer is 'yes' to the first two questions above, the chemical is assigned a Grade C_{dg}. The 'dg' indicates the chemical is assigned a Grade C based upon serious data gaps. If the answer to the third question is 'yes', the chemical is assigned a Grade F_{dg}. This communicates to the manufacturer that, although its chemical is initially assigned a Grade B, the final grade must be

adjusted based upon the importance of the data gaps. The chemicals final grade can be revisited once information is available to fill in the missing data.

Grade A: If a chemical has been assigned a Grade A based upon existing data, it is necessary to see if any data gaps could potentially adversely affect this grading. Based upon what data is missing, the following evaluations must be made:

- Does the chemical ranking table contain **one or more** data gaps for the following hazard endpoints: Carcinogenicity, Reproductive toxicity, Developmental Toxicity, Mutagenicity/Genotoxicity, Endocrine Activity, or Acute Mammalian Toxicity?
- Is the chemical ranking table contain a data gap for any of the following hazard criteria: Persistence, Bioaccumulation or Acute Aquatic Toxicity?

If the answer is ‘yes’ to the first question above, the chemical is assigned a Grade B_{dg}. The ‘dg’ indicates the chemical is assigned a Grade B based upon a data gap. If the answer to the second question is ‘yes’, the chemical is assigned a Grade F_{dg}. This communicates to the manufacturer that, although its chemical is initially assigned a Grade A, the final grade must be adjusted based upon the importance of the data gaps. The chemicals final grade can be revisited once information is available to fill in the missing data.

As can be observed from the above methodology, no chemical using the QCAT methodology can be assigned a Grade A if any data is missing. Just because a chemical has obtained a high grade using QCAT, a further review should be completed using a full GSTM analysis to be sure any of the missing criteria do not adversely affect its benchmark.

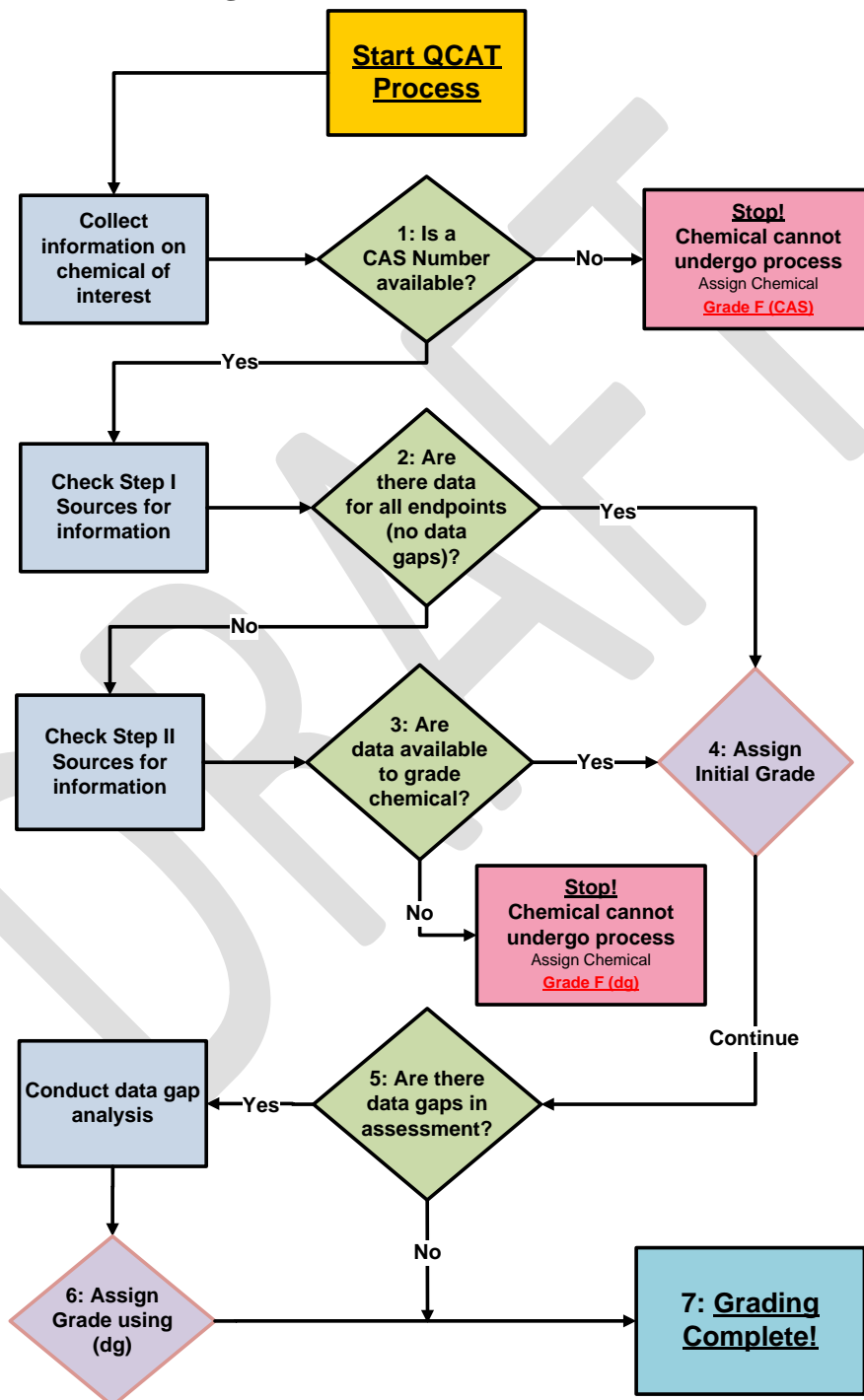
Results from the QCAT Grading Processes

Once the evaluation is complete for all the chemicals undergoing the QCAT review, the potential risks associated with each chemical can be compared directly. Those chemicals assigned Grade F should be removed from the manufacturing process. Safer alternatives should be sought for chemicals with a Grade C although they can be used while the search begins. Grade B chemicals still have some room for improvement but they are closer to being ‘green.’ Grade A chemicals are protective of human health and the environment based upon the QCAT review. A manufacturer may wish to subject these chemicals to the GSTM analysis to make sure that no unidentified hazard concerns exist. However, compared with other chemicals, Grade A chemicals do not pose a substantial risk for the priority endpoints used in the QCAT analysis.

4. QCAT Decision Logic

The QCAT decision logic used to determine the Grade for a chemical is depicted in Figure 1. The steps of the evaluation process are outlined below.

Figure 1 - QCAT Decision Logic



It is recommended that the same method be used to report results from the QCAT assessment as used for the GSTTM analysis. An example of a sample matrix is found in Appendix 3. Those hazard endpoints used in the GSTTM omitted from the QCAT are indicated as a question mark (?) for the QCAT assessment. In this manner, it is clear the results from the QCAT lack analysis of certain hazard endpoints used in the GSTTM and that, without this data, the uncertainty associated with the QCAT conclusions is greater.

The QCAT decision logic is based upon a six decision points that enable a user to complete the grading process. Before each decision point, data is collected which will assist the user in making the subsequent decision. Each decision point will be assigned a number and is described below with the data collection requirements preceding the decision point.

4. Start Quick Chemical Assessment Tool Process

Collect information on chemical of interest

In order to begin the evaluation process, it is important to collect some basic information on each chemical. Specifically, the following must be determined:

- Chemical name
- CAS number

If additional information is available, it may be advantageous to include it at this point. Other information of interest includes but is not limited to:

- Octanol/water coefficient (typically displayed as log K_{ow})
- Potential degradation products
- Uses

1: Is a CAS Number available?

A CAS number must be identified for each chemical to undergo the QCAT process. Without a CAS number, pertinent human health and environmental hazard data cannot be identified; therefore, a chemical without a CAS automatically exits the process and is assigned a provisional Grade F (CAS). This assessment may change as information is provided from manufacturers or EPA tightens its interpretation of confidential business information.

Check Step I data sources for QCAT hazard endpoints

Table 4 identifies the sources used in Step I for implementation of the QCAT. In Step I, the authoritative lists will be evaluated to determine if any of the chemicals undergoing evaluation appear on these authoritative sources. As indicated previously, several states and organizations

have established lists of chemical of concern that include many of the sources indicated in Step I. A user may wish to investigate these lists to see if any can be used in lieu of researching each individual source. See Appendix 1 for more details on these lists.

The sources in Step I are primarily simple lists and the evaluation depends on whether or not a chemical appears on the list. Some lists also provide information on the relative level of concern for the chemical based upon available data and review by technical experts. For example, EPA's Integrated Risk Information System (IRIS) database using 1986 criteria identifies chemicals that appear on their list as known, probable and possible carcinogens. It is important to include these details in the assessment results, as they will assist in the grading process.

Four simple databases have also been included in Step I sources. Information is provided at the end of Appendix 1 on how a user may access information in these databases and what data should be recorded for the grading process. At this point, all available information from the authoritative sources will be entered into the chemical matrix for each chemical.

2: Are there data for all hazard endpoints?

Once a table has been filled in with appropriate data from Step I sources (see Table 5 for an example table), it is important to determine if data have been found for all QCAT hazard endpoints. If data have been found to complete all hazard endpoints, it is not necessary to look at data from Step II sources.

Hazard endpoints identified in Step I data sources will not be evaluated further. Presence in any Step I source is deemed authoritative. Only those chemicals that do not appear in Step I sources will be subjected to further, Step II review. There is sufficient information to assign a final grade and the grading process jumps to decision #4.

Check Step II data sources for QCAT hazard endpoints

If any QCAT hazard endpoints remain blank after reviewing the data from Step I, it is necessary to research further for additional information using Step II data sources. Additional Step II data sources are identified in Appendix 2. The user should look only for data to fill in any remaining gaps. For example, if information was found in Step I sources for carcinogenicity, it is not necessary to look for similar information in Step II sources. The sources used in Step I are deemed authoritative and can be used directly in the grading process without further review or need for additional information.

Several databases in Step II are used to assist in assigning a hazard level to any remaining hazard endpoints. Guidance is provided at the end of Appendix 2 on how a user may access information in each database and what data should be recorded for the grading process.

The user should attempt to locate data from at least two Step II sources before ranking the chemical. If only one data source is found, the chemical can still be ranked using the information; however, it should be noted in the QCAT Report that further review might be warranted based upon the limited information available.

If after checking all the Step I and II data sources, information has not been found for one or more of the QCAT hazard endpoints, an 'DG' for 'data gap' is put into the matrix for that hazard endpoint(s). 'DG' indicates that, although all data sources were evaluated, no data have been found which would enable a level of concern to be assigned for this chemical for this specific hazard endpoint.

3: Is there data for any hazard endpoints that can be used to grade the chemical?

Once the table has been filled in with appropriate data from both Steps I and II sources and any data gaps have been identified, it is necessary to determine if data have been found for one or more of the hazard endpoints. If data have been found for one or more of the 9 hazard endpoints, it is possible to assess the data and begin the grading process as identified in #4.

If no data have been found using Step I and II sources, and only data gaps appear for all QCAT hazard endpoints, the chemical automatically exits the evaluation and is assigned a provisional grade 'F'. No further evaluation of this chemical occurs. Within the constraints of the QCAT system, this chemical is not a viable alternative to the toxic chemical being replaced. Data may exist for this chemical in sources not used by the QCAT, and a more detailed review using the GS™ process may identify this chemical as a viable alternative. This more detailed review is outside the scope of the QCAT.

4: Assign an Initial Grade to the chemical

The first step in this process is to determine the level of concern for each hazard endpoint using the data collected from the Step I and II sources. The level of concern ranges from very low for some hazard endpoints to very high for others. A simple color-coding system is used to identify a level of concern from very high (royal purple), high (red), moderate (yellow), low (light green) to very low (blue). Such color-coding is in agreement with the GS™ and assists in assigning an initial grade to the chemical.

These levels of concern can be identified using the process explained in Appendix 8. This

evaluation will produce a matrix with the level of concern filled in for all QCAT hazard endpoints, as shown in Table 5. It is recommended that you use a similar approach to display final results as is used in the GS™ as doing so demonstrates that this QCAT assessment is based upon fewer hazard endpoints than are included in a full GS™ assessment.

Table 6a: Example of assigned level of concern for each hazard endpoint

| Human - Group 1 | | | | | Human - Group 2 | | | | | | | Env. Health | | | Fate | | Physical | |
|-----------------|---|---|---|----|-----------------|----|---|-----|-----|-----|-----|-------------|----|----|------|----|----------|---|
| C | M | R | D | E | AT | ST | N | SnS | SnR | Irs | IrE | AA | CA | Eo | P | B | Ex | F |
| H | M | H | H | DG | vH | ? | ? | ? | ? | ? | ? | H | ? | ? | L | vL | ? | ? |

Once the levels of concern have been assigned for each hazard endpoint for which data were found, an initial grade is assigned to each chemical. This is accomplished using the process described on pages 12-13. The result of this evaluation will assign an ‘Initial Grade’ as shown in Table 6b.

Table 6b: Example of an initial grade assigned based upon the levels of concern identified.

Initial Grade

F

Data gaps are ignored at this point and a grade is assigned based solely upon what information is available for the chemical of interest. A further evaluation will review any data gaps to determine what level of confidence can be assigned to augment the initial grade.

5: Are there missing data for any hazard endpoints?

In order to better coordinate data requirements with existing regulatory requirements, a process has been established in the GS™ to evaluate chemicals for data gaps in important hazard endpoints. This process has been incorporated into the QCAT method. If ‘DG’ is found for one or more of the hazard endpoints, a further assessment is required.

Conduct a data gap analysis

Essentially, if a chemical undergoing the QCAT evaluation is missing data for one or more of the QCAT hazard endpoints, it is important to assess the impact these gaps may have upon the initial grade assigned using available data.

The ideal scenario would be to obtain sufficient data to assign a hazard level to each hazard endpoint. In reality there are chemicals for which there are no data for one or more hazard endpoints, and/or for which the manufacturer of the chemical is holding the data that has been generated as confidential business information.

The GS™ methodology Version 1.2 includes a data gap analysis. The intention of the data gap analysis and subsequent scoring is to promote and incentivize generation and disclosure of chemical hazard data. When data are missing and the hazard level for one or more hazard endpoints is unknown, a precautionary approach is taken when benchmarking the chemical. More complete data sets are required to achieve each subsequent benchmark score (from red to green).

In essence, the data gap analysis attempts to quantify the confidence in the initial grade assigned to each chemical. If data exists for all the hazard endpoints, the confidence is high that the impacts to human health and the environment can be correctly assessed. If there are important data gaps, the confidence in the assessment decreases substantially. The QCAT is guided by the most current version of the GS™ data gap analysis.

6: Assign a data gap grade to the chemical

The QCAT data gap process is very straightforward and is explained in more detail in the previous data gap section ([pages 13-15](#)). If a chemical is assigned an initial grade F based upon the data found, no data gap analysis is necessary as it is not possible for any data gaps to adversely impact this assessment. If, however, a chemical is assigned any grade higher than an F, the data gap analysis will attempt to quantify how confident we are in this assessment.

6: Grading Complete!

Congratulations! You have successfully completed the QCAT process. You can now summarize the grades assigned to all of the chemicals you have assessed using the QCAT. As part of the QCAT process, it is important to summarize the results of a QCAT evaluation for each chemical evaluated into a standardized format as shown in Appendix 6. The standardized format is based upon a similar report used to report the results from a GS™ evaluation. The details of the evaluation are documented and available for sharing with other interested parties. An example of a completed format for a QCAT evaluation is shown in Appendix 7.

It is important to understand how to interpret the grades. A chemical could receive a very high grade based upon what is known about it. However, if data on important priority endpoints are missing, there is less confidence that this grade actually reflects the potential impact the chemical may have upon human health and the environment.

Table 7 demonstrates these principles with a real life example. Ecology evaluated several chlorinated solvents against four fluorinated compounds that were being sold as safer alternatives. The two compounds listed in Table 7 are those that appear to have the lowest impact upon human health and the environment. Although the perfluorinated compound received the better grade (C versus F for the chlorinated compound), there is greater uncertainty about the grade as data for an important hazard endpoint (acute aquatic toxicity) is missing. It is impossible, therefore, to have a high level of confidence in the perfluorinated compound's initial grade, as this chemical may be toxic to the environment.

Although the chlorinated species received a lower grade 'F', data for all of the 6 priority endpoints are present for the chlorinated species. Only endocrine activity and carcinogenicity data are missing. The chlorinated species do have data for mutagenicity/genotoxicity, which can give an indication of whether these chemicals may be carcinogenic. Thus, the lack of a carcinogenicity study for the chlorinated species is not considered fatal to the evaluation.

In this example, the user may wish to explore other sources of information to see if any of the data gaps can be filled in or to contract with a toxicological service to see if the data gap can be filled in. Without this additional data, however, it is impossible to make a clear choice between the two options. It would be up to the final user to decide which chemical to use or, perhaps more appropriately, to explore whether there are other alternatives available which can be shown to have less of an impact upon human health and the environment.

Table 7: Example of two halogenated solvents

| | Human - Group 1 | | | | | Human - Group 2 | | | | | | | Eco | | | Fate | | Physical | |
|-------------|-----------------|---|---|---|----|-----------------|----|---|-----|-----|-----|-----|-----|----|----|------|----|----------|---|
| | C | M | R | D | E | AT | ST | N | SnS | SnR | Irs | IrE | AA | CA | Eo | P | B | Ex | F |
| Chlorinated | DG | L | L | L | DG | M | ? | ? | ? | ? | ? | ? | M | ? | ? | vH | vL | ? | ? |
| Fluorinated | L | L | L | L | DG | L | ? | ? | ? | ? | ? | ? | DG | ? | ? | vH | vL | ? | ? |

| | | Grade | |
|-------------|--|---------|-----------------|
| | | Initial | Final |
| Chlorinated | | C | C |
| Fluorinated | | B | F _{dg} |

The QCAT does allow incremental improvements, which may be necessary until data for all hazard endpoints become available. For example, you have two chemicals that have obtained Grades B and C respectively, based upon the data available. However, after you conduct the data gap analysis, you see that the chlorinated compound has received a Grade C and the fluorinated compound a Grade F_{dg} due to data gaps.

If you were to make a decision between these two chemicals to determine which might be a safer alternative based upon the initial Grade, it would appear the fluorinated compound is a safer choice, i. e. it is more reasonable to select the chemical that has a B grade over the chemical with a Grade C. However, upon further review of the data gaps, it is found that very important information is missing for the fluorinated compound, and that selection of the fluorinated alternative is actually risky due to the lack of important data. Until data on all the QCAT endpoints are available, however, there is no way to avoid the risk of making a choice about a chemical of unknown hazard. Thus, it is important to include data gaps in the evaluation.

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Appendix 1: Step I Data Sources

Individual Databases:

As mentioned previously, internet resources have been or are being made available that accumulate information from many of the Step I lists into a single site. These sites may potentially make a Step I evaluation easier for QCAT users. Detailed information on how to access each of these sites and obtain data that can be used in a QCAT evaluation can be found later in this appendix. The four sites potentially of interest to QCAT users are:

1. The Public Library of Materials (Plum), The University of California at Berkeley-The Berkeley Center for Green Chemistry
Source: <http://plm.berkeley.edu/>
2. The Interstate Chemicals Clearinghouse (IC2), IC2 State Priority Chemicals Resource database
Source: <http://www.newmoa.org/prevention/ic2/projects/resource/>
This seems to just list data sources, but no data....not sure helpful for QCAT purposes?
3. Healthy Building Network's Pharos Database's Chemical and Material Library
Source: <http://www.pharosproject.net/material/>
4. The WerCS Green Chemistry Scoring GreenScreen LiTe (GSL™)
Source: <http://www.TheWerCS.com/applications/green-chemistry-scoring>

In addition to these publicly available databases, QCAT also includes three databases compiled by government sources. These databases collect information on specific chemicals although the breadth of information is likely more limited than the four previous sources. The government databases included in QCAT are:

1. The European Commission's Joint Research Centre European Chemical Substances Information System (ESIS)
2. **Source:** <http://esis.jrc.ec.europa.eu/>
3. KEMI, Swedish Chemical Agency's N-Class Database providing risk phrase information on environmental hazard classification.
Source: <http://apps.kemi.se/nclass/>

Details on these seven databases and how to access information they contain are found below.

The user should take care to check when the information on these websites has been updated. Any site that is several years out-of-date should be used with caution. However, if a chemical was identified as a problem in one of the lists included in these sites, it is likely the chemical should be avoided and eliminated as viable safer alternative.

Authoritative Lists:

Authoritative lists for the above endpoints identified in Table 3 are provided below. Few authoritative government lists currently exist for neurotoxicants, vPTs and vBTs and endocrine disruptors. For endocrine disruptors, the available government lists are preliminary screening lists that identify chemicals which are prime candidates for the high concern label; however, these chemicals are in need of further assessment before they can be identified as endocrine disruptors with certainty. The same can be said for neurotoxicants. Grandjean and Landrigan (2008) have identified 201 chemicals that appear to be developmental toxicants. These chemicals also require further research to determine if they pose a developmental threat. Since neurotoxicity and endocrine activity are endpoints of high concern, these “watch” lists are provided as they flag chemicals that may meet these criteria. While these chemicals are under assessment, precautionary avoidance is warranted.

It is important to note that the authoritative lists are based on evaluation of only a limited set of the approximately 80,000 chemicals in commerce. Many chemicals have simply not been tested. Therefore it is important to assess the available toxicological literature on chemicals, which are not listed, and to use modeling tools and analogs to determine whether the weight of evidence indicates that a chemical is a chemical of high concern. The authoritative and watch lists that follow provide a starting point for identifying chemicals of high concern.

For the purposes of the QCAT, information will be selected from specific lists and from a few, easily accessible databases, which require no interpretative requirements. Information from these specialized databases will be described at the end of this appendix.

Human Health: Carcinogenicity

1. US National Institutes of Health, National Institute of Environmental Health Sciences, National Toxicology Program (NTP), 12th Report on Carcinogens (ROC)
 - a. Known to be Human Carcinogens
 - b. Reasonably Anticipated to be Human Carcinogens

Source: <http://ehis.niehs.nih.gov/roc>

2. US Environmental Protection Agency (EPA), National Center for Environmental Assessment, Integrated Risk Information System (IRIS) Database

- a. 1999 and 2005 Guidelines:
- b. Carcinogenic to humans
- c. Likely to be carcinogenic to humans
- d. 1996 Guidelines: “Known/likely human carcinogen
- e. 1986 Guidelines:
 - i. Group A - Human Carcinogen
 - ii. Group B1 - Probable human carcinogen
 - iii. Group B2 - Probable human carcinogen
 - iv. Group C - Possible human carcinogen

Source: http://www.epa.gov/ncea/iris/search_human.htm

3. International Agency for Research on Cancer (IARC), Agents Reviewed by the IARC Monographs

- a. Group 1: Agent is carcinogenic to humans
- b. Group 2A: Agent is probably carcinogenic to humans
- c. Group 2B: Agent is suspected carcinogenic to humans

Source: <http://monographs.iarc.fr/ENG/Classification/index.php>

4. State of California Environmental Protection Agency, Office of Environmental Health Hazard Assessment (OEHHA) California Proposition 65 (Safe Drinking Water and Toxic Enforcement Act Of 1986) Chemicals Known to the State to Cause Cancer or Reproductive Toxicity

Source: http://www.oehha.ca.gov/prop65/prop65_list/files/P65single111811.pdf

5. European Commission, Enterprise and Industry DG, Carcinogens List – See consolidated version of Annex I of Directive 76/769 EEC, which includes Annex I of Directive 65/548/EEC (which is to be replaced by Annex XVII of REACH on 1 June 2009).

- a. Carcinogen Category 1: “known”
- b. Carcinogen Category 2: “should be considered carcinogenic to humans”

Source: http://ec.europa.eu/enterprise/chemicals/legislation/markrestr/index_en.htm

6. Regulation on the Classification, Labeling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent amendments. Originally published in ECB, Annex I of Directive 67-548-EEC and subsequent amendments/adaptations, known as the Dangerous Substances Directive (DSD) or Directive on Dangerous Substances (DDS) EU CMR, Table 3.1 and similar information:

- a. Carc 1A
- b. Carc 1B
- c. Carc 2
- d. Category 1
- e. Category 2
- f. Category 3

Source #1: <http://ec.europa.eu/enterprise/sectors/chemicals/documents/classification/>
Data Found in Annex VI, Tables 3-1 & Table 3-2

Source #2: <http://www.reach-compliance.eu/english/legislation/docs/launchers/launch-annex-1-67-548-EEC.html>

7. National Institute for Occupational Safety and Health (NIOSH) Carcinogen List
Source: <http://www.cdc.gov/niosh/topics/cancer/npotocca.html>
8. The European Commission's Joint Research Centre European Chemical Substances Information System (ESIS) for EU risk phrases, if available.
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>
8. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.
Source: http://www.safe.nite.go.jp/english/ghs_index.html#results
9. European Chemical Agency's (ECHA) list of carcinogens identified in the Candidate List of Substances of Very High Concern (SVHC) for authorization.
Source: http://echa.europa.eu/chem_data/authorisation_process/candidate_list_table_en.asp

Human Health: Mutagenicity/Genotoxicity

1. European Commission, Enterprise and Industry DG, Mutagens List – See consolidated version of Annex I of Directive 76/769 EEC, which includes Annex I of Directive 65/548/EEC (which is to be replaced by Annex XVII of REACH on 1 June 2009).
 - a. Category 1
 - b. Category 2
 - c. Category 3
 - d. Muta 1A
 - e. Muta 1B
 - f. Muta 2

Source #1: <http://ec.europa.eu/enterprise/sectors/chemicals/documents/classification/>
Data Found in Annex VI, Tables 3-1 & Table 3-2

Source #2: <http://www.reach-compliance.eu/english/legislation/docs/launchers/launch-annex-1-67-548-EEC.html>
2. The European Commission's Joint Research Centre's European Chemical Substances Information System (ESIS) for EU Risk phrases, if available.
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>
3. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.
Source: http://www.safe.nite.go.jp/english/ghs_index.html#results

4. European Chemical Agency's (ECHA) list of mutagens identified in the Candidate List of Substances of Very High Concern (SVHC) for authorization.

Source: http://echa.europa.eu/chem_data/authorisation_process/candidate_list_table_en.asp

Human Health: Reproductive toxicity

Note to user: *These data sources are often the same as needed for Developmental, so check for both at the same time.*

1. European Commission, Enterprise and Industry DG, Mutagens List – See consolidated version of Annex I of Directive 76/769 EEC, which includes Annex I of Directive 65/548/EEC (which is to be replaced by Annex XVII of REACH on 1 June 2009).
 - a. Repro 1A
 - b. Repro 1B

Source #1: <http://ec.europa.eu/enterprise/sectors/chemicals/documents/classification/>
Data Found in Annex VI, Tables 3-1 & Table 3-2

Source #2: <http://www.reach-compliance.eu/english/legislation/docs/launchers/launch-annex-1-67-548-EEC.html>

1. State of California Environmental Protection Agency, Office of Environmental Health Hazard Assessment (OEHHA) California Proposition 65 (Safe Drinking Water and Toxic Enforcement Act Of 1986), Chemicals Known to the State to Cause Cancer or Reproductive Toxicity

Source: http://www.oehha.ca.gov/prop65/prop65_list/Newlist.html

2. US National Institutes of Health, National Institute of Environmental Health Sciences, National Toxicology Program (NTP), Health Assessment and Translation (Formerly CERHR). NTP-OHAT Monographs on the Potential Human Reproductive and Developmental Effects,

Source: <http://ntp.niehs.nih.gov/?objectid=974B2C24-030F-D308-60E11D088F83FADB>

3. The European Commission's Joint Research Centre's European Chemical Substances Information System (ESIS) for EU risk phrases, if available.

Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>

4. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.

Source: http://www.safe.nite.go.jp/english/ghs_index.html#results

5. European Chemical Agency's (ECHA) list of chemicals 'toxic for reproduction' identified in the Candidate List of Substances of Very High Concern (SVHC) for authorization.

Source: http://echa.europa.eu/chem_data/authorisation_process/candidate_list_table_en.asp

Human Health: Development (including developmental neurotoxicity)

1. State of California Environmental Protection Agency, Office of Environmental Health Hazard Assessment (OEHHA) California Proposition 65 (Safe Drinking Water and Toxic Enforcement Act Of 1986), Chemicals Known to the State to Cause Cancer or Reproductive Toxicity
Source: http://www.oehha.ca.gov/prop65/prop65_list/Newlist.html
2. US National Institutes of Health, National Institute of Environmental Health Sciences, National Toxicology Program (NTP), Health Assessment and Translation (Formerly CERHR). NTP-OHAT Monographs on the Potential Human Reproductive and Developmental Effects,
Source: <http://ntp.niehs.nih.gov/?objectid=974B2C24-030F-D308-60E11D088F83FADB>
3. The European Commission's Joint Research Centre's European Chemical Substances Information System (ESIS) for EU risk phrases, if available.
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>
4. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.
Source: http://www.safe.nite.go.jp/english/ghs_index.html#results
5. Grandjean, P & PJ Landrigan, 2006. "Developmental neurotoxicity of industrial chemicals." List of 201 chemicals with evidence suggesting developmental neurotoxicity in humans.
Source: *The Lancet*, v.368: 2167-2178.
9. Regulation on the Classification, Labeling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent amendments. Originally published in ECB, Annex I of Directive 67-548-EEC and subsequent amendments/adaptations, known as the Dangerous Substances Directive (DSD) or Directive on Dangerous Substances (DDS)
 - a. Developmental (EU CMR)**Source:** <http://ec.europa.eu/enterprise/sectors/chemicals/documents/classification/>

Human Health: Endocrine activity

Endocrine Disruptors Screening List. Chemicals listed in the European Union documents below are potential chemicals of concern. Precautionary avoidance is warranted.

1. European Union, Category 1 ("at least one in-vivo study providing *clear evidence* for endocrine activity in at least one species using intact animals"), Endocrine Disruptor chemicals. SCREENING LISTS –still undergoing assessment.
Sources:

- a. DHI. 2007. Study on Enhancing the Endocrine Disrupter Priority List with a Focus on Low Production Volume Chemicals.
http://ec.europa.eu/environment/endocrine/documents/final_report_2007.pdf
 - b. Commission Staff Working Document on the implementation of the "Community Strategy for Endocrine Disrupters" - a range of substances suspected of interfering with the hormone systems of humans and wildlife (COM (1999) 706), (COM (2001) 262) and (SEC (2004) 1372) (Brussels, 5 December 2007).
<http://register.consilium.europa.eu/pdf/en/07/st16/st16123.en07.pdf>
 - c. European Commission, Endocrine Disruptor Database.
http://ec.europa.eu/environment/endocrine/strategy/substances_en.htm#priority_list
2. Oslo-Paris Convention (OSPAR), Chemicals of Possible Concern identified as potential endocrine disruptors.
Source:
http://www.ospar.org/content/content.asp?menu=00950304450000_000000_000000

Human Health: Acute Mammalian Toxicity

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk phrases, if available.
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>
2. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.
Source: http://www.safe.nite.go.jp/english/ghs_index.html#results

Environmental Health: Acute Aquatic Toxicity

1. Canadian Environmental Protection Agency Domestic Substances List (DSL), DSL substances that are Inherently Toxic in the environment.
Source: <http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F>
2. Japanese Government National Institute of Technology and Evaluation (NITE) for estimated Risk Phrases, if available.
Source: http://www.safe.nite.go.jp/english/ghs_index.html#results
3. The European Commission's Joint Research Centre's European Chemical Substances Information System (ESIS) for EU risk phrases, if available.
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=cla>
4. KEMI, Swedish Chemical Agency's N-Class Database providing risk phrase information on environmental hazard classification.
Source: <http://apps.kemi.se/nclass/>

There are currently very few authoritative lists available for acute aquatic toxicity. Some additional compounds are present in the EPA List of Lists (see Acute Mammalian Toxicity above) because of their aquatic toxicity. As these chemicals are also assumed to have mammalian toxicity, they are not called out separately here.

As additional authoritative lists of chemicals with acute aquatic toxicity become available, they will be added to the QCAT. Until that point, there are other Step II data sources available, which will allow identification of acute aquatic toxicity for the QCAT.

Environmental Fate: Persistent, Bioaccumulative and Toxic (PBT) Substances¹³

1. United Nations Environment Programme (UNEP), Stockholm Convention Secretariat Stockholm Convention on Persistent Organic Pollutants (POPs)
Source: For the list of 12 POPs under the convention, see:
<http://chm.pops.int/Convention/12POPs/tabid/296/language/en-US/Default.aspx>;
Source: The list of 9 new POPs, see:
<http://chm.pops.int/Convention/ThePOPs/ThenewPOPs/tabid/2511/Default.aspx>
Source: For chemicals in review process, see:
<http://chm.pops.int/Convention/ThePOPs/Chemicalsproposedforlisting/tabid/2510/Default.aspx>
2. US Environmental Protection Agency (EPA), Toxics Release Inventory (TRI) Program, “TRI PBT Chemical List”
Source: http://www.epa.gov/triinter/trichemicals/pbt%20chemicals/pbt_chem_list.htm
3. US Environmental Protection Agency (EPA), Persistent Bioaccumulative and Toxic (PBT) Chemical Program, Priority PBT Profiles
Source: <http://www.epa.gov/opptintr/pbt/pubs/cheminfo.htm>
4. The European Commission’s Joint Research Centre’s European Chemical Substances Information System (ESIS) PBT list
Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=pbt>
5. State of Washington, Department of Ecology, Chapter 173-333 WAC Persistent Bioaccumulative Toxins
Source: <http://apps.leg.wa.gov/WAC/default.aspx?cite=173-333-310>
6. Oslo-Paris Convention (OSPAR), Chemicals of Possible Concern.
Source:
http://www.ospar.org/content/content.asp?menu=00950304450000_000000_000000
7. OSPAR, Chemicals for Priority Action.

¹³ Note: These are lists of chemicals which meet **both** the persistent and bioaccumulative requirements of the Quick Scan. If a chemical appears on these lists, they are **high** for both the bioaccumulation and persistence QS hazard endpoints.

Source:

http://www.ospar.org/content/content.asp?menu=00940304440000_000000_000000

8. Canadian Environmental Protection Agency Domestic Substances List (DSL), Persistent, Bioaccumulative and inherently Toxic chemical (PB_iT).

Source: <http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F>

9. European Chemical Agency's (ECHA) list of PBTs identified in the Candidate List of Substances of Very High Concern (SVHC) for authorization.

Source: http://echa.europa.eu/chem_data/authorisation_process/candidate_list_table_en.asp

Environmental Fate: very Persistent and very Bioaccumulative (vPvB) Substances¹⁴

1. European Chemical Agency's (ECHA) list of very persistent, very bioaccumulative (vPvB) chemicals identified in the Candidate List of Substances of Very High Concern (SVHC) for authorization.

Source:

http://echa.europa.eu/chem_data/authorisation_process/candidate_list_table_en.asp

Environmental Fate: Persistence

1. Canadian Environmental Protection Agency Domestic Substances List (DSL), Persistent and inherently Toxic chemical (PT).

Source: <http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F>

Environmental Fate: Bioaccumulation

1. Canadian Environmental Protection Agency Domestic Substances List (DSL), Bioaccumulative and inherently Toxic chemical (B_iT).

Source: <http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1&wsdoc=D031CB30-B31B-D54C-0E46-37E32D526A1F>

¹⁴ Note: These are lists of chemicals which meet **both** the persistent and bioaccumulative requirements of the QS. If a chemical appears on these lists, they are **very high** for both the bioaccumulation and persistence QS hazard endpoints.

Examples of Data from Individual Databases used in Appendix 1

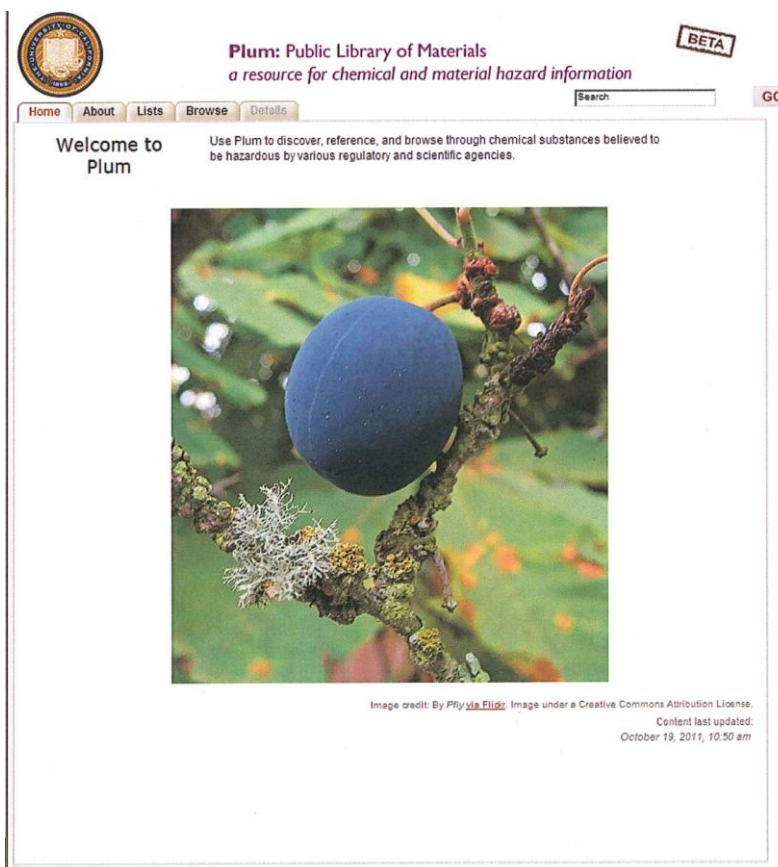
The Public Library of Materials (Plum): Plum contains a large amount of information on individual chemicals compiled from many of the lists in Step I sources. Plum currently contains chemicals identified by the following lists:

- Canadian Domestic Substances (DSL)
- Substitute It Now (SIN)
- European Commission PBT Information System
- REACH Annex VII Restricted Substances
- REACH Substances of Very High Concern (SVHC) Candidates
- International Agency for Research on Cancer (IARC) Monographs
- Stockholm Convention Persistent Organic Pollutants (POP)
- California Proposition 65 (Prop 65)
- Washington State Persistent, Bioaccumulative and Toxic (PBTs)
- Grandjean and Landrigan Neurotoxins
- European Commission Endocrine Disruptors (ED)
- Association of Occupational and Environmental Clinics (AOEC) Asthmagens
- US NIOSH Occupational Carcinogens

All except the SIN and AOEC lists are included in or relevant to QCAT Step I sources. If your chemical of interest is included in any of the other lists, the information can be used to grade chemicals.

Accessing Data in Plum:

The introductory page to Plum appears as:




One important piece of information to note on this page is the date that the contents were last updated, which was October 19, 2011 in the above example. Make sure to note this date on any assessment that you conduct.

You can access the information in Plum by inserting a name or CAS number into the 'Search' box. For the purposes of demonstrating Plum, the CAS number for formaldehyde (50-00-0) was inserted into this box. The results of the search appear as:

The screenshot shows the Plum: Public Library of Materials website. At the top, there is a logo on the left, the title "Plum: Public Library of Materials" with the subtitle "a resource for chemical and material hazard information", a "BETA" badge, and a "New Search" input field with a "GO" button. Below the title is a navigation bar with links: Home, About, Lists, Browse, and Details. The main content area is divided into three sections. The left section, titled "Click on one of the links below to further limit your view of items in Plum.", contains two categories: "Category" with a link to "Has CASRN ID 1" and "Listing Classification" with a link to "Select Multiple". The middle section, titled "PLUM currently has 1 substances, filtered by the following criteria:", shows a text search for "50-00-0" and a "Text search:" input field. The right section, titled "Search Results", shows a table with one row: "50-00-0" under "Substance ID" and "Formaldehyde" under "Name".

This information demonstrates that formaldehyde was identified in six lists, four of which are pertinent to QCAT, specifically the Prop 65, Canadian DSL, IARC and NIOSH cancer lists. The user can access more information on the specific chemical by clicking on the Substance ID value (50-00-0) highlighted above.

If you click on this link, the following information appears:

 **Plum: Public Library of Materials**
a resource for chemical and material hazard information

Home About Lists Browse Details

Formaldehyde

Name Variants (CASRN: 50-00-0)

The names of different substances sometimes vary in different data sources used by Plum. As a convenience, Plum automatically chose the shortest name variant for the title of this Web page. Alternate names and their source lists are provided below:

- Formaldehyde
Source: [Canada DSL](#), [SRI List 1.1](#), [IARC Monographs](#), [US NIOSH Occupational Carcinogen List](#)
- Formaldehyde (gas)
Source: [California Prop 65](#)
- Formaldehydes; Formalin
Source:

Accession into Plum:

Created: June 10, 2011
Last Updated: October 19, 2011
Link to: [Access Substances](#)

Substance Listing Information

Canada Domestic Substances List [\[More\]](#)

Categorized Potential Health Hazard
No
Human Health Priority
Low
Categorized Potential Environmental Hazard
No
Persistent
No
Bioaccumulative
No
Toxic to Aquatic Organisms
Yes
Categorized for further attention
No
Chemical Type
Organic
Listed Date
2005-05-05

Canada DSL

SRI List 1.1

Substitute & Now List (version 1.1) [\[More\]](#)

Reason for listing

Substitute & Now List (version 1.1) [\[More\]](#)

Reason for listing
Equivalent level of concern
Listed Date
2005-05-17

IARC Monographs

IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans [\[More\]](#)

IARC Classification
Group 1: Carcinogenic to humans
IARC Monographs Volume
68, 100F
Latest IARC Monographs Volume Hyperlink
<http://monographs.iarc.fr/HTML/index.php>
Listing documentation (link)
<http://monographs.iarc.fr/HTML/monographs/vol68/mono68-5.pdf>
Listed Date
2011-06-09

California Prop 65

California Proposition 65 List: Chemicals known to the state to cause cancer or reproductive toxicity [\[More\]](#)

Toxicity Type
cancer
No Significant Risk Level (HSRL) (µg/day)
40
Maximum Allowable Dose Level (MADL) (µg/day)
None
Listed Date
1985-01-01

Asthmagens on the ADEC Exposure Code List

ADEC Asthmagens [\[More\]](#)

Designated Asthmagens
Yes
ADEC Asthmagens classification
Generally accepted as asthmagens
ADEC Exposure Code
120.03

US NIOSH Occupational Carcinogen List

NIOSH Occupational Carcinogens [\[More\]](#)

Note
This authority has listed this substance

Information pertinent to a QCAT assessment for this chemical include:

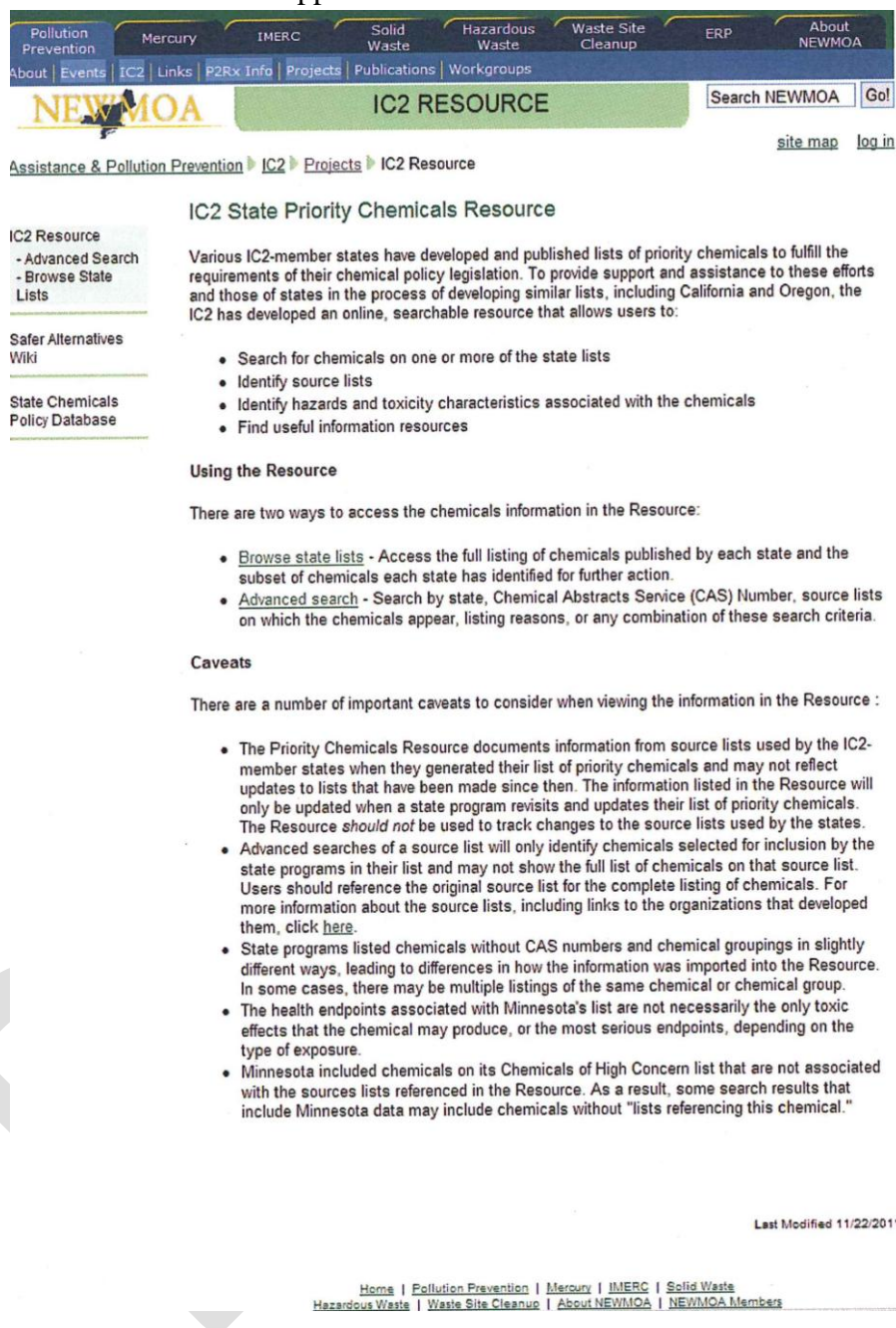
1. Toxic to Aquatic Organisms (Canadian DSL)
2. Group 1: Carcinogenic to humans (IARC)
3. Carcinogenic (Prop 65)
4. Carcinogen (NIOSH)

This information can be used to identify the level of concern for carcinogenicity and potentially for aquatic toxicity. The QCAT user should note this information in the assessment for formaldehyde and should make note of where the information was obtained (i.e. the Plum database accessed on a specific date.)

The Interstate Chemicals Clearinghouse (IC2) Database:

The IC2 assembled information used by three states (ME, MN and WA) that each state used to identify chemicals of concern. These lists were created as part of a response to legislation that was passed in each state to identify chemicals of potential concern to children, a subset of society specifically vulnerable to chemicals and their impact on human health and development. This information was made available for anyone interested in the sources of the chemicals identified by each state and may be useful to the QCAT users.

Initial access to the IC2 Database appears as:



Pollution Prevention Mercury IMERC Solid Waste Hazardous Waste Waste Site Cleanup ERP About NEWMOA

About Events IC2 Links P2Rx Info Projects Publications Workgroups

NEWMOA

IC2 RESOURCE

Search NEWMOA Go!

[site map](#) [log in](#)

[Assistance & Pollution Prevention](#) [IC2](#) [Projects](#) [IC2 Resource](#)

IC2 State Priority Chemicals Resource

Various IC2-member states have developed and published lists of priority chemicals to fulfill the requirements of their chemical policy legislation. To provide support and assistance to these efforts and those of states in the process of developing similar lists, including California and Oregon, the IC2 has developed an online, searchable resource that allows users to:

- Search for chemicals on one or more of the state lists
- Identify source lists
- Identify hazards and toxicity characteristics associated with the chemicals
- Find useful information resources

Using the Resource

There are two ways to access the chemicals information in the Resource:

- [Browse state lists](#) - Access the full listing of chemicals published by each state and the subset of chemicals each state has identified for further action.
- [Advanced search](#) - Search by state, Chemical Abstracts Service (CAS) Number, source lists on which the chemicals appear, listing reasons, or any combination of these search criteria.

Caveats

There are a number of important caveats to consider when viewing the information in the Resource :

- The Priority Chemicals Resource documents information from source lists used by the IC2-member states when they generated their list of priority chemicals and may not reflect updates to lists that have been made since then. The information listed in the Resource will only be updated when a state program revisits and updates their list of priority chemicals. The Resource *should not* be used to track changes to the source lists used by the states.
- Advanced searches of a source list will only identify chemicals selected for inclusion by the state programs in their list and may not show the full list of chemicals on that source list. Users should reference the original source list for the complete listing of chemicals. For more information about the source lists, including links to the organizations that developed them, [click here](#).
- State programs listed chemicals without CAS numbers and chemical groupings in slightly different ways, leading to differences in how the information was imported into the Resource. In some cases, there may be multiple listings of the same chemical or chemical group.
- The health endpoints associated with Minnesota's list are not necessarily the only toxic effects that the chemical may produce, or the most serious endpoints, depending on the type of exposure.
- Minnesota included chemicals on its Chemicals of High Concern list that are not associated with the sources lists referenced in the Resource. As a result, some search results that include Minnesota data may include chemicals without "lists referencing this chemical."

Last Modified 11/22/2011

[Home](#) | [Pollution Prevention](#) | [Mercury](#) | [IMERC](#) | [Solid Waste](#)
[Hazardous Waste](#) | [Waste Site Cleanup](#) | [About NEWMOA](#) | [NEWMOA Members](#)

As with Plum, the QCAT user should identify the date the database was last modified. Care should be taken though that this day agrees with the last time the data sources were updated in the database.

The Database allows users to either search for specific chemicals or to browse individual state lists. The information most useful to the QCAT user would be to conduct an 'Advance Search'. The 'Advance Search' pages appears as follows:

NEWMOA **IC2 RESOURCE** [Search NEWMOA](#) [Go!](#)
[site map](#) [log in](#)

[Assistance & Pollution Prevention](#) [IC2](#) [Projects](#) [IC2 Resource](#) [Advanced Search](#)

IC2 Resource
Advanced Search
Browse State Lists

Priority Chemicals Resource Advanced Search

Choose values from the fields below. Select multiple fields to narrow your search.

State

☐ Maine Department of Environmental Protection
☐ Minnesota Department of Health
☐ Washington State Department of Ecology

CAS Number - Hold control while you click to select multiple values

No CAS Number
50-00-0
50-05-6
50-07-7
50-18-0

You can also search by CAS number using the text box below. Separate multiple numbers with commas:

Chemical Name - Enter part or all of a chemical's name

Source List - To search a source list that includes multiple sub-lists, you must keep all sub-list check boxes selected. Selecting the source list check box and removing the sub-list check boxes will return no chemical records.

For more detailed information about these lists and links to the organizations that developed them, click [here](#) (PDF).

☐ California's Proposition 65 Program
☐ Canadian Environmental Protection Act Domestic Substances List - Persistent, Bioaccumulative, and Inherently Toxic Chemicals
☐ EPA Integrated Risk Information System
☐ EPA National Waste Minimization Program - Priority Chemicals
☐ EPA Persistent, Bioaccumulative, and Toxic (PBT) Chemicals Program - Priority PBT Chemicals
☐ EPA Toxics Release Inventory Program - Persistent, Bioaccumulative, and Toxic (PBT) Chemicals
☐ EPA Voluntary Children's Chemical Exposure Program
☐ European Commission - Directive on Dangerous Substances
☐ European Commission - Existing Substances Registration List
☐ European Commission Endocrine Disruptors
☐ European Union - Persistent, Bioaccumulative and Toxic Chemicals
☐ European Union - Substances of Very High Concern
☐ Grandjean and Landrigan Neurotoxins
☐ International Agency for Research of Cancer
☐ National Toxicology Program

The QCAT user can search the database either by CAS or name and can limit the search to either specific state lists or specific source lists. For the purposes of this example, a search will be based solely upon a specific CAS. As in the case of Plum, the CAS for formaldehyde (50-00-0) will be used. The results appear as:

The screenshot shows the NEWMOA IC2 DATABASE website. The top navigation bar includes links for Pollution Prevention, Mercury, IMERC, Solid Waste, Hazardous Waste, Waste Site Cleanup, ERP, and About NEWMOA. Below this is a secondary navigation bar with links for About, Events, IC2, Links, P2Rx Info, Projects, Publications, and Workgroups. The main header features the NEWMOA logo and the text 'IC2 DATABASE' with a search bar. The breadcrumb trail reads: Assistance & Pollution Prevention > IC2 > Projects > IC2 Resource > Chemical Detail. The left sidebar contains links to IC2 Resource, Advanced Search, and Browse State Lists. The main content area is titled 'Chemical Detail' and 'Formaldehyde (50-00-0)'. It provides additional information about the chemical, states that list it, and lists on which it resides. The footer includes a copyright notice for 2012 NEWMOA and contact information.

Information from this source is similar to what was found in Plum although additional information is provided as well. The information from this listing pertinent to a QCAT assessment includes:

1. Carcinogen (Prop 65)
2. Carcinogen (EPA IRIS)
3. Known Carcinogen (IARC)
4. Category B 'reasonably anticipated carcinogen' (NTP)

This information can be used to assign a level of concern for carcinogenicity for formaldehyde. The QCAT user should note the source and data this information was obtained and proceed with the QCAT assessment.

Healthy Building Network's Pharos Database:

As mentioned previously, Pharos is a subscription site and may not be available to all users. Costs for access, however, are reasonable and access to the information in Pharos might justify

the expense. Although Pharos was created primarily to improve the quality of building products, the data it contains will be useful for QCAT users. Users login to Pharos through its main page:

The screenshot shows the Pharos website interface. At the top, there is a navigation bar with the Pharos logo on the left and a user status bar on the right that says "happy sunday! free trial today? already a subscriber... login!". Below the navigation bar is a search bar with social media icons for Facebook, Twitter, and LinkedIn. The main content area is titled "Chemical and Material Library" and features a sub-header "the signal news & notes | building product library | chemical and material library | evaluation framework". The main heading is "Chemical and Material Library" with a sub-header "There are 12197 materials profiled in the Chemical and Material Library". Below this is a dark blue box with the text "Reduce your project's environmental and health hazards." and a list of bullet points: "Search over 10,000 substances screened against over 30 authoritative hazard and warning lists" and "View prioritized environmental and health hazards, restrictions, and potential health hazards in the life cycle". To the right of this is a green box with the text "Explore Pharos 15-day free trial". Below the main heading is a section titled "Search Made Simple" with a list of bullet points: "Search chemicals, wood species, and other materials by common name, scientific name, or CAS number" and "Autocomplete offers chemical selections as you type". To the right of this is a section titled "Chemical and Material Library" with a search bar that says "Search for a chemical, compound, or biobased material". Below the search bar is a section titled "Identify Direct Hazards" with a list of bullet points: "Chemicals, polymers, and other substances are screened against 26 hazard lists", "Wood species are screened against 5 endangered species lists", "All substances are also screened against 5 restricted substance lists", and "Health Hazards prioritization is informed by the GreenScreen for Safer Chemicals". To the left of this is a section titled "Discover Life Cycle Chemical Concerns" with a list of bullet points: "Pharos researches the manufacturing chemistry for substances in Pharos listed products, and these manufacturing chemicals are also screened for hazards" and "The Library identifies chemical residuals from the manufacturing process that may contaminate products." Below this is a section titled "How It Works:" with a sub-header "The Library identifies health hazards that may come directly from exposure to a substance or from chemicals used or created in the production or life cycle of this substance." and a list of bullet points: "Pharos researches the manufacturing chemistry for substances in Pharos listed products, and these manufacturing chemicals are also screened for hazards" and "The Library identifies chemical residuals from the manufacturing process that may contaminate products." To the right of this is a section titled "Lifecycle Hazard Quickscreen" with a sub-header "Research Status: Preliminary literature review drafted" and a list of bullet points: "The Pharos team has undertaken a preliminary literature review of some of the products and identified the following chemicals. This list of chemicals is not intended to be exhaustive of the production or life cycle of this substance." and a table with two columns: "Hazard Category" and "Chemical Name". The table lists the following chemicals: "PHthalic Anhydride [85-44-9] - Integral Monomer", "PHthalic Anhydride [85-44-9] - Integral Monomer", "PHthalic Anhydride [85-44-9] - Integral Monomer", "Sulfuric Acid [7664-93-9] - Frequent Catalyst", and "PHthalic Anhydride [85-44-9] - Integral Monomer".

Information in the upper right gives users access to the login page:

Pharos

happy sunday! [free trial today?](#) already a subscriber... [login!](#)

the signal news & notes | building product library | chemical and material library | evaluation framework

Login

Email Address

Password

Remember me on this computer. ☐

[Login](#)

[about pharos](#) | [contact us](#) | [terms of use](#) | [disclaimer](#) | [copyright information](#) | [privacy policy](#)

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Once access to the site is obtained, the following page appears:

[home](#) > [chemical and material library](#)

chemical and material library

Chemical and Material Library

There are 10639 substances in the library.

Enter the name or CAS registry number of a chemical, polymer, plant species or other material:

For chemicals, the Library identifies health hazards that may come from exposure to the material itself or from chemicals associated with its production.

For biobased materials, the Library identifies species that are endangered or may come from forest habitats that are threatened.

Click on the Chemical Hazard tab or Endangered Species tab for further explanation of each.

Chemical Hazards

Endangered Species

The Library identifies potential health hazards from both direct exposure to chemicals and from the releases of associated chemicals throughout the life cycle:

- **Direct health hazards:** Pharos screens materials against authoritative hazard listings to identify potential health hazards for those exposed to the material. Persistent bioaccumulative toxicants (PBTs) receive the highest priority for elimination followed by priority health effects: cancer, genetic mutation, reproductive or developmental harm and endocrine disruption.
- **Life cycle health hazards:** The Pharos team researches key materials to identify additional chemicals used, created and emitted throughout the material's life cycle. Pharos screens these chemicals to identify potential health hazards to the workers and local communities near where the raw materials are mined or grown and then manufactured into products.

Pharos staff conducts a preliminary literature review of life cycle chemicals for each ingredient of a Pharos listed product and more in-depth research on select common ingredients. Each chemical record is a work-in-progress. We welcome submissions and suggestions to improve our life cycle hazard data.

Pharos uses CAS registry numbers to compare materials against the Chemical Hazard lists in the box on the right side of the screen. If the material is listed, the name of the list and any warnings associated with that CAS number will be displayed along with a Pharos flag. Flags are color coded to indicate the Pharos system's prioritization of concern based upon the type of hazard and the degree of scientific evidence:

- Black - Urgent concern due to known persistence, bioaccumulation & toxicity (PBT) or extreme global warming or ozone depletion potential. Avoid immediately.
- Red - Very high concern due to known or probable cancer, mutation, endocrine disruption or reproductive or developmental harm, or very high global warming or ozone depletion potential. High priority to eliminate.
- Orange - High concern due to possible chronic toxicity, respiratory sensitization, ecotoxicity or high global warming or ozone depletion potential. Next priority for substitution.
- Yellow - Moderate concern due to acute health effects or moderate ecotoxicity, global warming or ozone depletion or preliminary data of higher concern health effects. Avoid when possible.
- Blue - This substance has been identified for avoidance or careful management on a Restricted Substance List (RSL).

Details

Chemical Hazard Lists

Total Lists Scanned: 25

AOEC Asthmagens

Association of Occupational and Environmental Clinics

CAL-EPA Prop 65

State of California Environmental Protection Agency, Office of Environmental Health Hazard Assessment (OEHHA)

ECHA REACH SVHC

European Union - European Chemicals Agency

European Commission Directive 76/769 CMR

European Commission, Enterprise and Industry DG

European Commission Endocrine Disruptors Strategy

European Commission, Council of the European Union DG ENV

Biobased Warning Lists

Total Lists Scanned: 5

FOE Good Wood Guide

Friends of the Earth

IUCN Red List

International Union for Conservation of Nature and Natural Resources (IUCN)

UNEP WCMC CITES-listed Trees

United Nations Environment Programme - World Conservation Monitoring Centre (WCMC)

USDA US Threatened & Endangered Trees

US Department of Agriculture, Natural Resources Conservation Service

WWF Tropical Wood Guide

World Wildlife Federation

Total Lists Not Scanned: 1

Restricted Substance List

Total Lists Scanned: 6

Cascadia Living Building Red List

Cascadia Region Green Building Council and International Living Building Institute

EU ROHS

European Union

P-W Precautionary List

Perkins+Will

Using formaldehyde as an example, the CAS number 50-00-0 is entered into Pharos and the following information appears:



chemical and material library

Enter chemical, polymer, CAS registry number or bio based material to find a

match:

[Details](#)

FORMALDEHYDE

CAS RN: 50-00-0

[Show products that contain this material](#)

| PBT | Carcinogen | Mutagen | Reproductive | Developmental | Endocrine | Other Chronic | Acute | Ecotoxicant | Action List |
|-----|------------|---------|--------------|---------------|-----------|---------------|-------|-------------|-------------|
| — | KNOWN | — | — | — | — | KNOWN | KNOWN | — | KNOWN |

Compound Groups

[FORMALDEHYDE BASED COMPOUNDS](#) [CMG10502] [▼](#)

Direct Hazard Warnings

Total warnings for FORMALDEHYDE: 14

1986 Guidelines Group B1: Probable human carcinogen: based on limited evidence of carcinogenicity in humans and sufficient evidence of carcinogenicity in animals
US Environmental Protection Agency, National Center for Environmental Assessment (US EPA NCEA)
Integrated Risk Information System Database (IRIS Carcinogens)

Group 1: Agent is carcinogenic to humans
International Agency for Research on Cancer, World Health Organization (IARC)
Monographs On the Evaluation of Carcinogenic Risks to Humans (Cancer Monographs)

Cancer
State of California Environmental Protection Agency, Office of Environmental Health Hazard Assessment (OEHHA) (CAL-EPA)
Chemicals Known to the State to Cause Cancer or Reproductive Toxicity - California Proposition 65 - Safe Drinking Water and Toxic Enforcement Act Of 1986 (Prop 65)

Known to be Human Carcinogens
US Dept of Health & Human Services, National Institutes of Health, National Institute of Environmental Health Sciences, National Toxicology Program (US NIH NTP)
12th Report on Carcinogens (RoC)

▣ **R40: Limited evidence of a carcinogenic effect**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)
Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

▣ **AG: known asthmagen - generally accepted**

Association of Occupational and Environmental Clinics (AOEC)
AOEC Exposure Code List (Asthmagens)

▣ **Listed Hazardous Air Pollutant**

US Environmental Protection Agency, Technology Transfer Network (US EPA TTN)
Clean Air Act Amendments of 1990 List of Hazardous Air Pollutants (HAPs)

▣ **R23: Toxic by inhalation.**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)
Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

▣ **R24: Toxic in contact with skin.**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)
Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

▣ **R25: Toxic if swallowed.**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)
Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

■ **R34: Causes burns.**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)

Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

■ **R43: May cause sensitization by skin contact.**

European Commission, Joint Research Centre, Institute for Health and Consumer Protection,
Consumer Products Safety & Quality Unit (European Commission)

Substances with EU Risk & Safety Phrases (Commission Directive 67-548-EEC) (Risk Phrases)

■ **OSHA Carcinogen listed**

US EPA & US Department of Labor, Occupational Safety and Health Administration (US OSHA)

TRI Carcinogens (Carcinogens)

■ **Red List of Chemicals to Avoid in LBC Projects**

Cascadia Region Green Building Council and International Living Building Institute (Cascadia)

Living Building Challenge 2.0 - Red List of Materials & Chemicals (Living Building Red List)

Life Cycle (chemicals used or emitted in the life cycle of FORMALDEHYDE)

This list of chemicals is not exhaustive of all chemicals that may be involved in the production or life cycle of this substance.

METHANOL [67-56-1] ■ ■ ■ ■ ■ ■ ■ ■ ■ ■

- **Role in manufacture:** Integral Feedstock.
- **Emitted during manufacture:** Unknown. No known data or unclear data.
- **Exposure in use:** Unknown. No known data or unclear data.
- **Exposure in degradation:** Unknown. No known data or unclear data.
- **Exposure in combustion:** Unknown. No known data or unclear data.

SILVER [7440-22-4] ■ ■

- **Role in manufacture:** Frequent Catalyst.
- **Emitted during manufacture:** Unknown. No known data or unclear data.
- **Exposure in use:** Unknown. No known data or unclear data.
- **Exposure in degradation:** Unknown. No known data or unclear data.
- **Exposure in combustion:** Unknown. No known data or unclear data.

FERRIC OXIDE [1309-37-1] ■

- **Role in manufacture:** Occasional/rare Catalyst.
- **Emitted during manufacture:** Unknown. No known data or unclear data.
- **Exposure in use:** Unknown. No known data or unclear data.
- **Exposure in degradation:** Unknown. No known data or unclear data.
- **Exposure in combustion:** Unknown. No known data or unclear data.

COPPER [7440-50-8] ■ ■ ■

- **Role in manufacture:** Occasional/rare Catalyst.
- **Emitted during manufacture:** Unknown. No known data or unclear data.
- **Exposure in use:** Unknown. No known data or unclear data.
- **Exposure in degradation:** Unknown. No known data or unclear data.
- **Exposure in combustion:** Unknown. No known data or unclear data.

Information pertinent to a QCAT assessment for this chemical includes:

1. Group B1 using 1986 Guidelines (IRIS)
2. Group 1: Carcinogenic to humans (IARC)
3. Carcinogenic (Prop 65)
4. Known to be a human carcinogen (NTP RoC)
5. Carcinogen (OSHA)
6. R40, Limited evidence of a carcinogenic effect, GHS risk phrase (ESIS)
7. R25, Toxic if swallowed, GHS risk phrase (ESIS)

This information can be used to identify the level of concern for carcinogenicity and acute mammalian toxicity. The QCAT user should note this information in the assessment for formaldehyde and should make note of where the information was obtained (i.e. the Pharos database accessed on a specific date.)

It is also important to note that Pharos includes data from sources used in the GSTM but not in QCAT and information that is meaningful to its target audience, i. e. suppliers of building materials. Although there is a temptation to include this information in a QCAT assessment, it is outside the scope of the QCAT and should be reserved for a GSTM assessment.

GreenScreenTM LiTe (GSL):

The GSLTM is still under development and information on its contents is still in the draft stage. However, once completed, users will be able to enter their products into The WerCS system and select a GSLTM review. A table will appear summarizing results for each chemical in the product similar to what is found in the QCAT and GSTM methods. The chemical will also be assigned a benchmark based upon the data. The following is an example of a possible GSLTM report format:

WERCS Studio - Microsoft Internet Explorer provided by The WERCS, Ltd

http://wercsdevws02-vm/WerCS.GreenScreen.Web/GSPProduct.aspx?MODELID=1&PRODUCT=RM00001

Green Screen Assessment Tool

Amit Test Product With supplier Association (RM00001)

Hazard Table

View Published Assessment

Product Benchmark

Lowest Scoring constituent: 1
Scoring by weight Percent:

| Percent in formula | Benchmark |
|--------------------|-----------|
| 25 | 1 |

Chemical

| | % Formulation | Benchmark | Priority Effects | | | Health Effects | | | Ecotox. | Fate. | P-Chm | | | | | | | |
|--|---------------|-----------|------------------|---------------------------|---------------|----------------|-----------|--------------------|---------|-------|-------|-----------------|---------------|---------------|------------------------|----------------|----------------|------------------|
| | | | Carcinogenicity | Mutagenicity/Genotoxicity | Rep. Toxicity | Dev. Toxicity | Endocrine | Dev. Neurotoxicity | | | | Acute Mam. Tox. | Sys. Toxicity | Sensitization | Irritation/Corrosivity | Immunotoxicity | Acute Aq. Tox. | Chronic Aq. Tox. |
| Chemical Formulation | | | | | | | | | | | | | | | | | | |
| 100-17-44-Nitroanisole Add/Edit Doc | 10 | | | | | | | | | | | | | | | | | |
| 100-20-9/Terephthaloyl chloride Add/Edit Doc | 15 | 1 | H | M | | | | | | | | | | | | | | |
| 104-15-4/p-Toluenesulfonic acid Add/Edit Doc | 5 | 1 | H | M | L | DG | H | | | | | | | | | | | U |
| 3319-31-1/TEHTM Add/Edit Doc | 15 | | U | U | U | U | | | | | | | | | | | | |
| 7440-38-2/Arsenic Add/Edit Doc | 5 | 1 | H | M | H | H | | | | | | | | | | | | |
| 93384-43-1/Toxins, botulin, A Add/Edit Doc | 5 | | | | | | | | | | | | | | | | | |
| Transformation Product | | | | | | | | | | | | | | | | | | |
| Delete 100-21-0/Terephthalic acid | - | | | | | | | | | | | | | | | | | |
| Delete 100-33-4/Pentamidine | - | | | | DG | | | | | | | | | | | | | |
| Delete 7732-18-5/Water, distilled, conductivity or of similar purity | - | | | | | | | | | | | | | | | | | |

Refresh Hazard Table

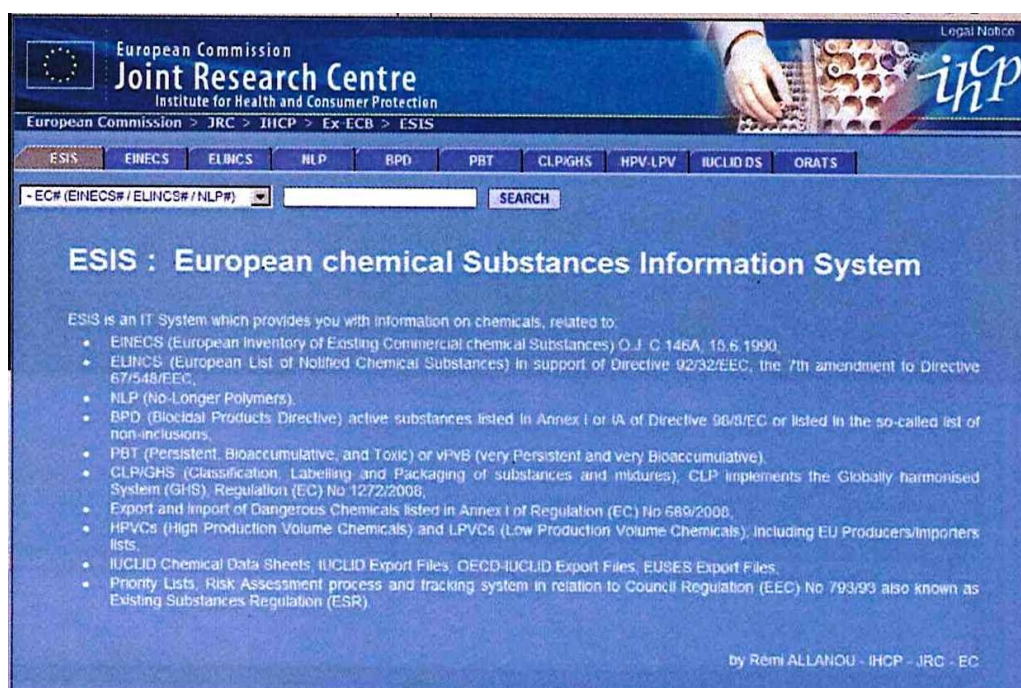
Back Preview Assessment Finalize Assessment

Local intranet | Protected Mode: Off

CPA and The WerCS hope to have this system finalized within the next few months. Any questions about the final version should be directed to The WerCS, which can be found on the internet at: <http://www.TheWerCS.com/applications/green-chemistry-scoring>. Potential users should be reminded, however, that there is a subscription cost to access The WerCS services; therefore, the information above may only be useful to those users who have already paid for services from The WerCS.

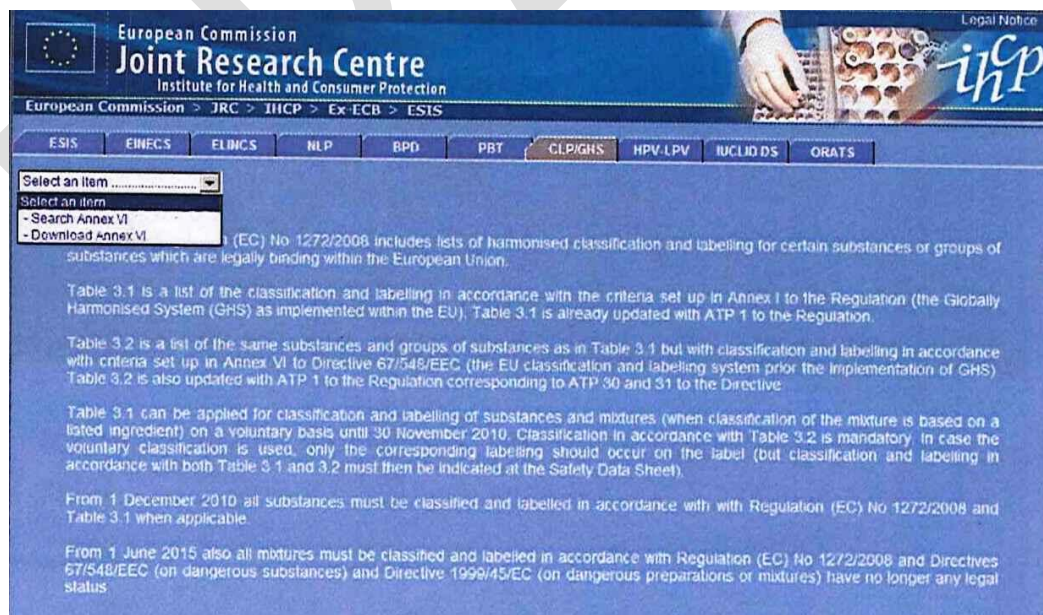
European Chemical Substances Information System (ESIS): ESIS contains a large amount of information on individual chemicals including documents such as risk assessments, OECD Substance Information Data Sheets (SIDS), etc. For the QCAT Step I review, however, the information to be used is the Classification and Risk Phrases displayed on the section labeled CLP/GHS (for classification and labeling program/global harmonization system).

The main page of ESIS appears as follows:



Each tab represents specific information on chemicals collected or required by the European Union. For the purposes of the QCAT Step I review, the tab labeled CLP/GHS contains the most useful information.

The CLP/GHS tab appears as follows:



It is necessary to 'select an item' to identify what information is of interest. Although it is possible to download the list with complete information, it is typically easier just to search for

information on a specific chemical or, in this case, 'Search Annex VI'.

The CLP/GHS tab then changes to appear as follows:

The screenshot shows the 'Search Annex VI' form on the European Commission Joint Research Centre website. The form is titled 'Search Annex VI to Regulation (EC) No 1272/2008 on Classification, Labelling and Packaging of Dangerous Substances'. It includes a search bar with the text 'Search Annex VI' and a dropdown menu. Below the search bar, there are several input fields: 'Language' (set to EN), 'Index number', 'EC number', 'CAS number', and 'Substance Name'. There are also two dropdown menus for 'Risk Phrases' (showing R2, R3, R4, R5, R6) and 'Hazard Statement Codes' (showing EUH059, H200, H201, H203, H220). The 'ATP' field is set to 'ALL'. The form has a 'Search' button and a 'Clear' button.

The only information needed at this point is the CAS number. Although the database gives the user the option of selecting specific risk phrases or hazard codes, this is not recommended unless the user is very familiar with either the CLP or GHS.

Using formaldehyde (CAS 50-00-0) as an example, the CAS is entered and the 'Search' button selected. The following information is displayed.

ESIS (European chemical Substances Information System) - Windows Internet Explorer

http://ecoweb3.jrc.it/esis/index.php?PGM=cds

European Commission
Joint Research Centre
Institute for Health and Consumer Protection

European Commission > JRC > IHCP > EX-ECB > ESIS

ESIS ENFCS ELBCS NLP BPD PBT CLP/GHS HPV/LPV IUCLID DS ORATS

Search Annex VI

Details on Substances Classified in Annex VI to Regulation (EC) No 1272/2008

| General Information | | | |
|---------------------|------------------------------|-----------|----------------------------|
| Index number | Notes (alphabetic / numeric) | | ATP inserted / ATP updated |
| | Table 3.1 | Table 3.2 | |
| 005-001-00-5 | B D / - | B D / - | CLP00 / - |

| Sub | EC No | Cas No | Name |
|-----|-----------|---------|--------------|
| 1 | 200-001-6 | 50-00-0 | formaldehyde |

Regulation (EC) No 1272/2008 Annex VI Table 3.1

| Classification | Hazard Statement Code(s) | Pictogram Signal Word Code(s) | Hazard Statement Code(s) | Suppl. Hazard statement code(s) |
|----------------|--------------------------|-------------------------------|--------------------------|---------------------------------|
| Carc. 2 | H351 | GHS08 | H351 | |
| Acute Tox. 3 * | H331 | GHS09 | H331 | |
| Acute Tox. 3 * | H311 | GHS09 | H311 | |
| Acute Tox. 3 * | H301 | Dgr | H301 | |
| Skin Corr. 1B | H314 | | H314 | |
| Skin Sens. 1 | H317 | | H317 | |

| Concentration | Classification |
|----------------|---------------------|
| C ≥ 25 % | Skin Corr. 1B: H314 |
| 5 % ≤ C < 25 % | Skin Irrit. 2: H315 |
| 5 % ≤ C < 25 % | Eye Irrit. 2: H319 |
| C ≥ 5 % | STOT SE 3: H335 |
| C ≥ 0.2 % | Skin Sens. 1: H317 |


Regulation (EC) No 1272/2008 Annex VI Table 3.2

| Classification | Risk phrases | Safety phrases | Indication(s) of danger |
|-------------------|--------------|----------------|-------------------------|
| Carc. Cat. 3: R40 | 23/24/25 | 1/2 | T |
| T: R23/24/25 | 34 | 26 | |
| C: R34 | 40 | 36/37/38 | |
| R43 | 43 | 45 | |
| | | 51 | |

| Concentration | Classification |
|----------------|----------------|
| C ≥ 25 % | T: R23/24/25 |
| 5 % ≤ C < 25 % | Xn: R20/21/22 |
| C ≥ 25 % | C: R34 |
| 5 % ≤ C < 25 % | X: R36/37/38 |
| C ≥ 0.2 % | R43 |

| Seveso Data | | | | |
|-----------------------|----------------------|-------------------------|----------------------|------------|
| Seveso Substance | Main Seveso Category | Other Seveso Categories | Seveso Concentration | Categories |
| Yes (Named substance) | 0 | 2 | C ≥ 25 % | D-2 |
| | | | 5 % ≤ C < 25 % | - |
| | | | 1 % ≤ C < 5 % | - |
| | | | 0.2 % ≤ C < 1 % | - |

Symbol(s)

 Toxic

Back New Search

Table 3.1 lists information identified using criteria established under the GHS. Table 3.2 lists similar information used to comply with the EU's CLP. The QCAT relies heavily upon the classification system established by the GHS and this information should be used primarily to establish a level of concern. In instances where the CLP values are more conservative, it is recommended that the user take the more conservative approach and use the lower value.

In the example above, formaldehyde is identified as a category 2 carcinogen and an acute mammalian toxic chemical via exposure to the skin, lungs and digestive system. This

information satisfies two of the QCAT hazard endpoints.

Lastly, this source may include information on hazard criteria that are part of the GSTTM but are not included in the QCAT. In order to concentrate on those hazard criteria with the greatest impact upon human health and the environment, several hazard criteria are not included in the QCAT but are reserved for a more complete GSTTM analysis. If the user wishes to include this information in an assessment, it is recommended they use the GSTTM process as many data sources exist pertinent to these hazard endpoints are excluded from the QCAT.

KEMI Swedish Chemicals Agency N-Class Database on Environmental Hazards: The Swedish Chemicals Agency in collaboration with the European Chemicals Bureau has collected information on the environmental hazard classification for approximately 7,000 compounds and has provided this information in its N-Class Database. The introductory page for the database appears as follows:



A simple 'Substance search' sends you to a window where the name, CAS number or other defining information can be entered:

The screenshot shows the "Substance search menu". It has a title "- Substance search menu -" and two buttons at the top right: "Advanced Search" and "Go to Main menu". Below are four input fields with labels: "Name:" (with a hint "(Enter part of name)"), "CAS No:" (with a hint "(- beginning of No as by XXX-YY-Z)"), "EEC No:" (with a hint "(- beginning of No as by XXXYYZ)"), and "Aresen Index No:" (with a hint "(- beginning of No as by AEC-EAT-VW-Y)"). At the bottom right are two buttons: "Clear search" and "Search".

The database will then display whether or not the compound is found in the database:

- Substance search result - Hits: 1
Intermediate list Search string: [CAS No = 106-49-0*]

Please click on a CAS No. for more information on the substance.

| CAS No | Name | Synonym or Group Name |
|----------|-------------------------|-----------------------------|
| 106-49-0 | Benzeneamine, 4-methyl- | m-toluidine; 3-aminotoluene |

By selecting the information highlighted in blue, the data is displayed:

- Substance search result -

Back to the List Print a report Go to Main menu

| | | | |
|------------------------|--|------------------------|-------------------------|
| CAS No | 106-49-0 | Name | Benzeneamine, 4-methyl- |
| EEC No | 0054031 | Synonyms or Group Name | <ITAD>m<ITAD>-toluidine |
| Code No | 0005 | Annex I Index No | 012-024-00-4 |
| Aquatic classification | XN, R50 | Based on | Data |
| On-site classification | | | See 106-44-1 |
| Annex I classification | T, R23/24/25 R37 N, R50 | NTPC | ATP |
| Summary recorder | 10-12 May 1991 Meeting on environmental effects 13-14 October 1993 Meeting on environmental effects 20-22 June 1995 Meeting on environmental effects | | |
| Comments | ECBC 00 99-Rex 3 | | |

Application of Criteria

The GHS classification is provided in the box labeled 'Aquatic Classification.' Note that that additional information on other potential toxicity concerns may also be displayed in the box labeled 'Annex I classification.'

This source of aquatic information may prove useful to complete the QCAT.

Appendix 2: Step II data sources

For the purposes of the QCAT, the following databases will be searched for specific information, which can be used to grade chemicals undergoing the assessment process. Although considerable information is available from all of these sources, only specific information will be selected for review in support of the objectives of the QCAT to limit the level of technical expertise necessary. Information used from each database will be described in detail at the end of this appendix.

As in Step I sources, an additional database exists that accumulates information on many if not all of the hazard endpoints being evaluated in QCAT. At the end of 2011, the European Chemical Agency (ECHA) compiled all of the GHS data for chemicals submitted during registration as required under REACH.

ECHA has made no attempt to review the submittals and there may be errors within the database; however, as there is no incentive for a manufacturer to report a problem for a chemical if none exists, this database is potentially a good source for hazard data for chemicals that have been identified as containing some level of concern.

As the database has not been reviewed, there is less of a guarantee that chemicals within the database are correctly evaluated and there may be chemicals with hazard concerns that are not identified. QCAT users may wish to evaluate the information in this database for any data gaps remaining after evaluating other Step II sources. If a chemical is identified as a concern for any of the remaining hazard endpoints, the results can be used to define the degree of hazard involved. If there are any conflicts between this database and other Step II sources, the other sources should be given greater emphasis as this database has not been peer reviewed or audited.

The ECHA database can be found at:

1. European Chemicals Agency, Classification and Labeling Database (C&L Database).
Source: <http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database>

Information on how to access information within the database will be presented later in this appendix after the list of data sources for each individual hazard endpoint.

Human Health: Carcinogenicity

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: <http://esis.jrc.ec.europa.eu/index.php?PGM=dat>
2. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>

3. National Institute of Occupational Safety and Health (NIOSH), Registry of Toxic Effects of Chemical Substances (RTECS).
Source: <http://ccinfoweb.ccohs.ca/rtecs/search.html>
4. US Department of Labor, Occupational Safety & Health Administration (OSHA) Occupational Chemical Database.
Source: <http://www.osha.gov/web/dep/chemicaldata/default.asp>
5. ISSCAN: Instituto Superiore di Sanita, 'Chemical Carcinogens: Structures and Experimental Data'.
Source: http://epa.gov/comptox/dsstox/sdf_isscan_external.html
Additional Information: Found at *Data (file XLS)*: [ISSCAN v3a 1153 19Sept08.xls](#)
6. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDSEIDS/sidspub.html>

Human Health: Mutagenicity/Genotoxicity

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
Note: ESIS also provides links to other data sources that might prove useful including the IUCLID datasets. If this additional data exists, links will be found at the bottom of the ESIS page.
2. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>
3. National Institute of Occupational Safety and Health (NIOSH), Registry of Toxic Effects of Chemical Substances (RTECS).
Source: <http://ccinfoweb.ccohs.ca/rtecs/search.html>
4. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDSEIDS/sidspub.html>

Human Health: Reproductive toxicity

Note to user: These data sources are often the same as needed for Developmental, so check for both at the same time.

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>

IUCLID Source: http

2. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>
3. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDIDS/sidspub.html>

Human Health: Developmental toxicity (including Developmental neurotoxicity)

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: http
2. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>
3. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDIDS/sidspub.html>

Human Health: Endocrine activity

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
2. National Institute of Occupational Safety and Health (NIOSH), Registry of Toxic Effects of Chemical Substances (RTECS).
Source: <http://ccinfoweb.ccohs.ca/rtecs/search.html>

Human Health: Acute Mammalian Toxicity

1. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
RA Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: http ??
2. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>
3. National Institute of Occupational Safety and Health (NIOSH), Registry of Toxic Effects of Chemical Substances (RTECS).

Source: <http://ccinfoweb.ccohs.ca/rtecs/search.html>

4. Danish Ministry of the Environment's Environmental Protection Agency (Q)SAR Assessment of chemical properties of substances.
User Manual for the Internet Version of the Danish (Q) SAR Database

Source Background:

http://www.mst.dk/English/Chemicals/assessment_of_chemicals/qsar_assessment_chemical_properties_of_substances/

Database: <http://130.226.165.14/index.html>

5. The United Nation's Screening Information Datasets (SIDS), if available.

Source: <http://www.chem.unep.ch/irptc/sids/OECDSEIDS/sidspub.html>

Environmental Health: Acute Aquatic Toxicity

1. National Library of Medicine (NLM), Hazardous Substances Database (HSDB).
Source: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>
2. US Environmental Protection Agency, Ecological Toxicity (ECOTOX) database.
Source: <http://cfpub.epa.gov/ecotox/>
3. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: [http](http://)
4. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDSEIDS/sidspub.html>

Environmental Fate: Persistence

1. US Environmental Protection Agency, Ecological Toxicity (ECOTOX) database.
Source: <http://cfpub.epa.gov/ecotox/>
2. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: [http](http://)
3. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDSEIDS/sidspub.html>

Environmental Fate: Bioaccumulation

1. US Environmental Protection Agency, PBT Profiler.
Source: <http://www.epa.gov/oppt/sf/tools/pbtprofiler.htm>
2. US Environmental Protection Agency, Ecological Toxicity (ECOTOX) database.
Source: <http://cfpub.epa.gov/ecotox/>
3. European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) for EU risk assessments or the International Uniform Chemical Information Database (IUCLID) dataset, if available.
ESIS Source: <http://esis.jrc.ec.europa.eu/>
IUCLID Source: <http://www.eurochem.info/iuclid/>
4. The United Nation's Screening Information Datasets (SIDS), if available.
Source: <http://www.chem.unep.ch/irptc/sids/OECDSEDS/sidspub.html>

Examples of Data from Individual Databases used in Appendix 2

European Chemical Agency (ECHA) Classification and Labeling Database: As with other databases in Step II, the C&L database collects information on a wide range of chemicals. The database simply reports the information that ECHA has received and ECHA does not verify the accuracy of the information within the database.

Access to the C&L database is straightforward. The opening page appears as:



C&L Inventory database

This database contains classification and labeling information on notified and registered substances received from manufacturers and importers. It also includes the list of harmonised classifications.



Notifications and registrations which do not indicate a classification are not included in this release of the inventory (see C&L Inventory Q&A no. 2).

Further information:

[Dissemination website](#) to check if the substance is registered as non-classified.

[More information about the C&L Inventory](#)

[Video tutorial](#)

Learn the search functions and features of the public C&L Inventory

[Understanding the CLP Regulation](#)

Search Classification and Labelling Inventory

Search Criteria

Substance Name

☐ Starts with... ☒ Contains ☐ Matches exactly with...

Other Identifier

☐ Only Harmonised C&L

Classification Details

| | Hazard Class and Category Code(s) | Hazard Statement Code(s) |
|-----------------------|--|--|
| Physical hazards | <div>Diss. Gas Expl. 1.1 Expl. 1.2 Expl. 1.3</div> | <div>H200 H201 H202 H203</div> |
| Health Hazards | <div>Acute Tox. 1 Acute Tox. 2 Acute Tox. 3 Acute Tox. 4</div> | <div>H300 H301 H302 H303</div> |
| Environmental Hazards | <div>Aquatic Acute 1 Aquatic Acute 2 Aquatic Acute 3 Aquatic Chronic 1</div> | <div>EUH059 H400 H401 H402</div> |

You may select one or more of the above values by using the Control (CTRL) key.

☐ In order to perform a search you need to read through and agree to this [legal disclaimer](#).

Search

Clear

The QCAT user can search for information in several ways but the recommended method is to insert the CAS number in the line called 'Other Identifier'. The user MUST also check the small box at the end of the sentence 'In order to perform a search you need to read through and agree to this [legal disclaimer](#)'. Without checking this box, the user will not be able to proceed to the actual data.

Using formaldehyde as an example, the CAS number 50-00-0 is entered into the second line and the 'Search' button is pressed. Before pressing 'Search', the database would appear as follows:

Search Classification and Labelling Inventory

Search Criteria

Substance Name

☐ Starts with... ☒ Contains ☐ Matches exactly with...

Other Identifier

50-00-0

☐ Only Harmonised C&L

Classification Details

| | Hazard Class and Category Code(s) | Hazard Statement Code(s) |
|-----------------------|---|---|
| Physical hazards | <div>Diss. Gas</div> <div>Expl. 1.1</div> <div>Expl. 1.2</div> <div>Expl. 1.3</div> | <div>H200</div> <div>H201</div> <div>H202</div> <div>H203</div> |
| Health Hazards | <div>Acute Tox. 1</div> <div>Acute Tox. 2</div> <div>Acute Tox. 3</div> <div>Acute Tox. 4</div> | <div>H300</div> <div>H301</div> <div>H302</div> <div>H303</div> |
| Environmental Hazards | <div>Aquatic Acute 1</div> <div>Aquatic Acute 2</div> <div>Aquatic Acute 3</div> <div>Aquatic Chronic 1</div> | <div>EUH059</div> <div>H400</div> <div>H401</div> <div>H402</div> |

You may select one or more of the above values by using the Control (CTRL) key.

In order to perform a search you need to read through and agree to this [legal disclaimer](#). ☒

Search

Clear

The database will conduct a search for the requested information and identify any information that meets the desired criteria. The search on the CAS number for formaldehyde yields the following:


All of the entries contain the desired search criteria in one location or another. The QCAT user would click on the file in the 'View' column for the second line which coincides with the desired CAS number for formaldehyde, i.e. 50-00-0. Clicking on the link in 'View' causes the following information to be displayed:

Summary Of Classification and Labelling

Harmonised classification - Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation)

General Information

| EC Number | CAS Number | Index Number | International Chemical Identification |
|-----------|------------|--------------|---------------------------------------|
| 200-001-8 | 50-00-0 | 605-001-00-5 | formaldehyde ... % |

ATP Inserted / Updated: CLP00 
CLP Classification (Table 3.1)

| Classification | | Labelling | | | Specific Concentration limits, M-Factors | Notes |
|-----------------------------------|--------------------------|--------------------------|--|---------------------------------|---|--|
| Hazard Class and Category Code(s) | Hazard Statement Code(s) | Hazard Statement Code(s) | Supplementary Hazard Statement Code(s) | Pictograms, Signal Word Code(s) | | |
| Acute Tox. 3 * | H301 | H301 | | GHS06 GHS05 GHS08 Dgr | * STOT SE 3; H335: C ≥ 5% Skin Corr. 1B; H314: C ≥ 25% Skin Sens. 1; H317: C ≥ 0,2% Eye Irrit. 2; H319: 5% ≤ C < 25% Skin Irrit. 2; H315: 5% ≤ C < 25% | Note B Note D |
| Acute Tox. 3 * | H311 | H311 | | | | |
| Skin Corr. 1B | H314 | H314 | | | | |
| Skin Sens. 1 | H317 | H317 | | | | |
| Acute Tox. 3 * | H331 | H331 | | | | |
| Carc. 2 | H351 | H351 | | | | |

| Signal Words | Pictograms | | |
|--------------|--|---|--|
| Danger |  |  |  |
| | Skull and crossbones | Corrosion | Health hazard |

The database provides hazard codes for acute toxicity and carcinogenicity. If these hazard endpoints have been satisfied using data from Step I sources, this information may not be useful. As the database contains information on a wider range of chemicals than those identified in Step I sources, it is likely that information on other chemicals will prove more useful. This example, however, gives an indication of the type of information available and how it is displayed.







The database also provides other information that is not useful to most QCAT users. For example, the formaldehyde report includes information on specific types of reports that lead to the summary information above. This data appears as follows:

Notified classification and labelling

General Information

| EC Number | CAS Number | IUPAC Name  |
|-----------|------------|--|
| 200-001-8 | 50-00-0 | 13215_50-00-0 |

Notified classification and labelling according to CLP criteria

| Classification | | | Labelling | | Specific Concentration limits, M- Factors | Notes | Number of Notifiers  | Joint Entries  | View |
|-----------------------------------|--------------------------|--------------------------|--|--------------------------------|--|--|---|---|---|
| Hazard Class and Category Code(s) | Hazard Statement Code(s) | Hazard Statement Code(s) | Supplementary Hazard Statement Code(s) | Pictograms Signal Word Code(s) | | | | | |
| Acute Tox. 3 | H301 | H301 | | GHS06 GHS05 GHS08 Dgr | STOT SE 3: C ≥ 5% Skin Corr. 1B: C ≥ 25% Skin Sens. 1: C ≥ 0,2% Eye Irrit. 2: 5% ≤ C < 25% Skin Irrit. 2: 5% ≤ C < 25% | Note B Note D | 985 | |  |
| Acute Tox. 3 | H311 | H311 | | | | | | | |
| Skin Corr. 1B | H314 | H314 | | | | | | | |
| Skin Sens. 1 | H317 | H317 | | | | | | | |
| Acute Tox. 3 | H331 | H331 | | | | | | | |
| Carc. 2 | H351 | H351 | | | | | | | |
| Acute Tox. 3 | H301 | H301 | | GHS06 GHS05 GHS08 Dgr | | | 177 | |  |
| Acute Tox. 3 | H311 | H311 | | | | | | | |
| Skin Corr. 1B | H314 | H314 | | | | | | | |
| Skin Sens. 1 | H317 | H317 | | | | | | | |
| Acute Tox. 3 | H331 | H331 | | | | | | | |
| Carc. 2 | H351 | H351 | | | | | | | |
| Acute Tox. 3 | H301 | H301 | | GHS06 GHS05 GHS08 Dgr | STOT SE 3: C ≥ 5% Skin Corr. 1B: C ≥ 25% Skin Sens. 1: C ≥ 0,2% Eye Irrit. 2: 5% ≤ C < 25% Skin Irrit. 2: 5% ≤ C < 25% | Note B Note D | 93 |  |  |
| Acute Tox. 3 | H311 | H311 | | | | | | | |
| Skin Corr. 1B | H314 | H314 | | | | | | | |
| Skin Sens. 1 | H317 | H317 | | | | | | | |
| Eye Dam. 1 | H318 | | | | | | | | |
| Acute Tox. 3 | H331 | H331 | | | | | | | |
| Carc. 2 | H351 | H351 | | | | | | | |

As the data is summarized earlier, it is unlikely this information would prove useful to the standard QCAT user. It is mentioned here, however, so the QCAT user understands what is being displayed and whether or not it would be useful to review the report in more detail.

Hazardous Substances Database (HSDB): The HSDB contains considerable information on the toxicity of specific chemicals. This information includes excerpts from specific sources and detailed information on the specific impacts of the chemical. HSDB also displays specific toxicity results, which have undergone technical review and conclusions on certain toxicity criteria, which will be of use in a QCAT evaluation. The three primary toxicity criteria of interest are acute mammalian toxicity, acute aquatic toxicity and carcinogenicity. Information may be available on other toxicity criteria included in the QCAT; however, these data varies widely from chemical to chemical and should be used with caution.

Data on specific chemicals contain in the HSDB have the following general appearance:

The Table of Contents on the left displays various pages of the report. Data in three specific pages will be discussed in the subsequent sections.

Acute Mammalian Toxicity: Acute mammalian toxicity values of interest for the QCAT evaluation are typically displayed on the page labeled 'Non-human toxicity values.' Using formaldehyde as an example, HSDB displays the following information on the page labeled 'Non-human toxicity values':

FORMALDEHYDE CASRN: 50-00-0

Non-Human Toxicity Values:

LD50 Rat oral 100 mg/kg /SRP: percent solution not specified/

*[Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1814] **PEER REVIEWED***

LD50 Rat (albino) oral 2020 mg/kg /From table/ /SRP: percent solution not specified/

*[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001),, p. 5:967] **PEER REVIEWED***

etc.....

For the purposes of the QCAT, the toxicity values provided may prove useful.

Acute aquatic toxicity: Aquatic toxicity values of interest for the QCAT evaluation are typically displayed on the page labeled 'Ecotoxicity values.' Using formaldehyde as an example, HSDB displays the following information on the page labeled 'Ecotoxicity values':

FORMALDEHYDE

CASRN: 50-00-0

Ecotoxicity Values:

*LC50 /Morone saxatilis/ (Striped bass, larvae) 10 mg/L/48-96 hr; static bioassay
[Environmental Canada; Tech Info for Problem Spills: Formaldehyde p.67 (1985)]
PEER REVIEWED*

*LC50 Oncorhynchus mykiss (Rainbow trout, weight 0.63 g) 118 ppm/96 hr (95%
confidence limit: 99.7-140 ppm); static /37% AI formulated product/
[USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on
Formaldehyde (50-00-0). Available from, as of May 30, 2006:
http://cfpub.epa.gov/ecotox/quick_query.htm] **PEER REVIEWED***

etc....

For the purposes of ecotoxicity review, LC50 fish data will be evaluated using the process established within Washington State's Dangerous Waste Regulations (WAC 173-303)

'Fish LC₅₀ data must be derived from an exposure period greater than or equal to twenty-four hours. A hierarchy of species LC50 data should be used that includes (in decreasing order of preference) salmonids, fathead minnows, and other fish species.'

For other ecotoxicity data, the species with the most data are assumed to be indicative of the toxic effects for the chemical under review. This information can be directly applied to the QCAT grade criteria.

Carcinogenicity: The HSDB also where available provides an assessment of whether or not a chemical is a known or suspected carcinogen. Much of the information in this assessment is pulled from other sources used in the Step I analysis and may be duplicative. However, the HSDB does include other sources which may be useful in a Step II evaluation. For example, the carcinogenicity information on formaldehyde appears as:

FORMALDEHYDE

CASRN: 50-00-0

Evidence for Carcinogenicity:

Evaluation: There is sufficient evidence in humans for the carcinogenicity of formaldehyde. There is sufficient evidence in experimental animals for the

carcinogenicity of formaldehyde. Overall evaluation: Formaldehyde is carcinogenic to humans (Group 1).

[IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Vol 88 Summary of Data Reported and Evaluation. (Last updated: September 7, 2004). Available from, as of June 22, 2006:

*<http://monographs.iarc.fr/ENG/Monographs/vol88/volume88.pdf>] **PEER REVIEWED***

CLASSIFICATION: B1; probable human carcinogen. BASIS FOR CLASSIFICATION: Based on limited evidence in humans, and sufficient evidence in animals. Human data include nine studies that show statistically significant associations between site-specific respiratory neoplasms and exposure to formaldehyde or formaldehyde-containing products. An increased incidence of nasal squamous cell carcinomas was observed in long-term inhalation studies in rats and in mice. The classification is supported by in vitro genotoxicity data and formaldehyde's structural relationships to other carcinogenic aldehydes such as acetaldehyde. HUMAN CARCINOGENICITY DATA: Limited. ANIMAL CARCINOGENICITY DATA: Sufficient.

[U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS). Summary on Formaldehyde (50-00-0). Available from, as of March 15, 2000:

*<http://www.epa.gov/iris/>] **PEER REVIEWED***

A2; Suspected human carcinogen.

*[American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 31] **QC REVIEWED***

Formaldehyde: reasonably anticipated to be a human carcinogen.

[DHHS/National Toxicology Program; Eleventh Report on Carcinogens: Formaldehyde (50-00-0) (January 2005). Available from, as of July 31, 2009:

*<http://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/s089form.pdf>] **QC REVIEWED***

Three out of the four sources are used found in Step I although the conclusion from the American Conference of Governmental Industrial Hygienists TLVS and BEIs is not. This source was reviewed by experts and deemed worthy for inclusion. Additional sources like this might prove useful for other chemicals not identified in Step I sources.

Searching HSDB: An easier method for locating information in the HSDB is to click on the first page, which includes the complete record for the chemical being evaluated. This record can then be searched (by pressing the Control key and 'F' simultaneously) to search out pertinent information for each hazard criteria. Ecology has found the following keywords (or any portion thereof) useful in evaluating data contained in the HSDB:

- Carcinogenicity
- Mutagenicity
- Genotoxicity (used to report mutagenicity results)
- Reproduction
- Developmental

The user may use other keywords that assist in this process.

Registry of Toxic Effects of Chemical Substances (RTECS): RTECS contains data on several toxicity endpoints, which may be of interest to a GS™ evaluation. However, many of endpoints require technical expertise to evaluate prior to including in a safer chemical alternative assessment. For the purposes of the QCAT, the acute mammalian toxicity and tumorigenic/carcinogenicity data may prove useful.

Acute Mammalian Toxicity: The RTECS record for formaldehyde contains the following information for acute toxicity:

ACUTE TOXICITY DATA

| Type of Test | Route of Exposure | Species Observed | Dose Data | Toxic Effects | Reference |
|--|-------------------|------------------|-----------|---|---|
| LD50 - Lethal dose, 50 percent kill | Oral | Rodent - rat | 100 mg/kg | Details of toxic effects not reported other than lethal dose value | FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- Volume(issue)/page/year: 26,447,1988 |
| LC50 - Lethal concentration, 50 percent kill | Inhalation | Rodent - rat | 203 mg/m3 | Peripheral Nerve and Sensation - spastic paralysis with or without sensory change Behavioral - convulsions or effect on seizure threshold Behavioral - excitement | GTPZAB Gigiena Truda i Professional'nye Zabolevaniya. Labor Hygiene and Occupational Diseases. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) V.1-36, 1957-1992. For publisher information, see MTPEEI Volume(issue)/page/year: 18(2),55,1974 |
| etc..... | | | | | |

The RTECS acute toxicity dose data may prove useful in completing a QCAT evaluation.

Tumorigenic/Carcinogenicity: The RTECS record for formaldehyde contains the following information for tumorigenic toxicity:

TUMORIGENIC DATA

| Type of Test | Route of Exposure | Species Observed | Dose Data | Toxic Effects | Reference |
|------------------------------------|-------------------|------------------|---------------------------|---|--|
| TDLo - Lowest published toxic dose | Oral | Rodent - rat | 109 gm/kg/2Y (continuous) | Tumorigenic - <u>carcinogenic by RTECS criteria</u> ¹⁵ Gastrointestinal - tumors Blood - leukemia | TIHEEC Toxicology and Industrial Health. (Princeton Scientific Pub. Co., POB 2155, Princeton, NJ 08540) V.1- 1985- Volume(issue)/page/year: 5,699,1989 |

etc.....

The determination of whether or not a chemical is determined as tumorigenic/carcinogenic using RTECS criteria may prove useful in completing a QCAT evaluation.

Occupational Safety & Health Administration (OSHA) Occupational Chemical Database (OCD): The OCD contains information on the potential exposure concerns related to worker health and safety. Although the acute toxicity information requires considerable technical expertise, the OCD does identify chemicals as potential carcinogens.

The Exposure limits section of the report for formaldehyde contains the following information:

| Exposure Limits | | |
|-------------------|--------------------|---|
| OSHA | NIOSH | Related Information |
| PEL-TWA ppm: 0.75 | REL-TWA ppm: 0.016 | AIHA Emergency Response Planning Guidelines - ERPG-1/ERPG-2/ERPG-3: |
| PEL-TWA mg/m3: | REL-TWA mg/m3: NA | |

¹⁵ Emphasis added to show reviewer what information to use for making determination.

| | | |
|-----------------------------|---|--|
| NA | | 1 ppm/10 ppm/25 ppm |
| PEL-STEL ppm: 2 | REL-STEL ppm: NA | |
| PEL-STEL mg/m3: NA | REL-STEL mg/m3: NA | |
| PEL-C ppm: NA | REL-C ppm: 0.1 | |
| PEL-C mg/m3: NA | REL-C mg/m3: NA | Carcinogen Classifications: IARC-2A, NIOSH-Ca, NTP-R, OSHA-Ca, TLV-A2⁴ |
| Skin Notation: No | Skin Notation: No | |
| Notes: SEE 29 CFR 1910.1048 | Notes: CARCINOGEN (Ca)⁴; 15 MINUTE CEILING | |
| | IDLH ppm: 20 | |
| | IDLH mg/m3: NA | |
| | IDLH Notes: Ca | |

Although much of the information on carcinogenicity is pulled from sources used in Step I, additional information used to determine carcinogenicity may prove useful in completing a QCAT evaluation.

Ecological Toxicity (ECOTOX) database: ECOTOX is a major source of ecological toxicity information; however, unlike many of the previous sources, EPA does not conduct detailed technical review of all of the information included in ECOTOX and there will be more variability in the quality of data found within. To address some of these concerns, a ‘weight of evidence’ approach will be used to identify values to be used in a QCAT evaluation. In addition, the exposure hierarchy described in the HSDB section above (Salmonids followed by fathead minnow followed by any other fish species) will be used during data evaluation.

For example, ECOTOX record for formaldehyde contains approximately 100 acute aquatic toxicity (LC₅₀) entries for Rainbow Trout. The following is an excerpt of this data:

| <u>Spec. Sci. Name</u> <u>Spec. Common Name</u> | <u>Endpoint</u> <u>BCF</u> | <u>Effect</u> <u>Effect Meas.</u> | <u>Resp. Site</u> <u>Exp. Dur. (Days)</u> | <u>Conc (ug/L)</u> <u>Appl. Rate</u> | <u>Media Type</u> <u>Loc</u> | <u>Ref#</u> | <u>View Details</u> |
|--|-------------------------------|--------------------------------------|--|---|---------------------------------|-------------|------------------------------|
| Oncorhynchus mykiss Rainbow Trout | LC50 | MOR MORT | 1 | F 134000* (109000* - 164000*) ug/L | FW LAB | 7443 | View Details |
| Oncorhynchus mykiss | LC50 | MOR MORT | 1 | F 140000* (117000* - 167000*) ug/L | FW LAB | 7443 | View Details |

| | | | | | | | |
|---------------------|------|------|---|---------------------------------------|-----|------|------------------------------|
| Rainbow Trout | | | | | | | |
| Oncorhynchus mykiss | LC50 | MOR | | F 155000* (133000* - 182000*) ug/L | FW | 7443 | View Details |
| Rainbow Trout | | MORT | 1 | | LAB | | |
| Oncorhynchus mykiss | LC50 | MOR | | F 54000* (42000* - 69600*) ug/L | FW | 7443 | View Details |
| Rainbow Trout | | MORT | 1 | | LAB | | |

Many of the LC₅₀ results can be discarded because the test lasted less than 24 hours. The remaining tests which lasted anywhere from 1 to 4 days provided results ranging from 1,410 to 320,000 µg/L. However, the low values were found in a limited number of studies and a majority of the results were in the 100,000 to 200,000 µg/L range. Therefore a value of 150,000 micrograms per liter (equivalent to 150 mg/L) would be selected for the QCAT as being most representative of the data in ECOTOX.

ECOTOX also contains information on a chemical's bioaccumulation factor. For example, some of the record the BCF factors for shown below:

Report Generated: Sat Oct 30 13:50:40 2010

Aquatic Search Results: 1067 Records

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 Next>> References Page 1 of 16

| Spec. Sci. Name Spec. Common Name | Endpoint BCF | Effect Effect Meas. | Resp. Site Exp. Dur. (Days) | Exp. Type Chem. Anal. | Trend Eff % | Signif. Sig. Level | Conc (ug/L) Appl. Rate | Media Type Loc | Ref# | View Details |
|--------------------------------------|-----------------|------------------------|--------------------------------|--------------------------|----------------|-----------------------|---------------------------|-------------------|-------|------------------------------|
| Algae, Moss, Fungi | | | | | | | | | | |
| Chlorella vulgaris Green Algae | BCF 170 | ACC GACC | WO 0.014 | S U | | | T 1E-5 mol/L | FW LAB | 9927 | View Details |
| Chlamydomonas sp. Green Algae | BCF 210 | ACC GACC | WO 0.014 | S U | | | T 0.001 mol/L | FW LAB | 9927 | View Details |
| Chlorella vulgaris Green Algae | BCF 260 | ACC GACC | WO 0.014 | S U | | | T 0.001 mol/L | FW LAB | 9927 | View Details |
| Chlorella vulgaris Green Algae | BCF 260 | ACC RSDE | 0.014 | S U | INC | | T 207000 ug/L | FW LAB | 45149 | View Details |
| Chlamydomonas sp. Green Algae | BCF 330 | ACC GACC | WO 0.014 | S U | | | T 0.0001 mol/L | FW LAB | 9927 | View Details |
| Chlorella vulgaris Green Algae | BCF 690 | ACC GACC | WO 0.014 | S U | | | T 0.0001 mol/L | FW LAB | 9927 | View Details |
| Chlorella vulgaris Green Algae | BCF 690 | ACC RSDE | 0.014 | S U | INC | | T 20700 ug/L | FW LAB | 45149 | View Details |
| Chlamydomonas sp. Green Algae | BCF 920 | ACC GACC | WO 0.014 | S U | | | T 1E-5 mol/L | FW LAB | 9927 | View Details |
| Chlorella vulgaris Green Algae | BCF 1700 | ACC RSDE | 0.014 | S U | INC | | T 2070 ug/L | FW LAB | 45149 | View Details |
| Chlorella vulgaris Green Algae | BCF 1700 | ACC RSDE | 7 | S U | INC | | T 20700 ug/L | FW LAB | 45149 | View Details |

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 Next>> References Page 1 of 16

As with other information, the user must determine which BCF values to use. A 'weight of evidence' approach as shown in other examples in this document might be a preferred method. However, if bioaccumulation information cannot be found in the other sources or confirmatory values are needed, ECOTOX may prove a valuable source to determine whether or not a chemical bioaccumulates.

ISSCAN Chemical Carcinogens: Structures and Experimental Data: ISSCAN is an Italian database which contains information on carcinogen and mutagen potential based upon technical review of scientific studies and computer modeling input using Quality Structure Activity Relationship ((Q)SAR) processes. The information is provided in an Excel spreadsheet and information on both the carcinogenic and mutagenic potential is provided.

The data is presented in a range from 1 to 3 where:

- 3 = carcinogenic or mutagenic
- 2 = undetermined or equivocal.
- 1 = non-carcinogenic or non-mutagenic.

Some chemicals were not evaluated particularly for mutagenicity due to a lack of data and are identified as 'nd' for 'no data.'

For example, the ISSCAN provides the following information (additional detail excluded for the purposes of a QCAT review)

| ChemName | CAS | Canc | SAL ¹⁶ |
|----------------|---------|------|-------------------|
| Vinyl chloride | 75-01-4 | 3 | 3 |

Therefore for the purposes of the QCAT, vinyl chloride would be identified as a known carcinogen and known mutagen.

Access to the ISSCAN data is via an EPA website at:

http://epa.gov/comptox/dsstox/sdf_isscan_external.html. The EPA page appears as follows:

EPA United States Environmental Protection Agency

LEARN THE ISSUES | SCIENCE & TECHNOLOGY | LAWS & REGULATIONS | ABOUT EPA

ALL EPA THIS AREA Advanced Search

Computational Toxicology Research Program

You are here: EPA Home » Research & Development » CompTox » DSSTox

SDF Download Page

ISSCAN: Istituto Superiore di Sanita, "CHEMICAL CARCINOGENS: STRUCTURES AND EXPERIMENTAL DATA"

Brief Description: This database originates from the experience of researchers of the Environment and Primary Prevention Department in the field of structure-activity relationships (SAR), aimed at developing models which theoretically predict the carcinogenicity of chemicals. A portion of the chemicals has been the subject of carcinogenicity classification by various Regulatory Agencies and Scientific Bodies. The database has been specifically designed as an expert decision support tool and includes these carcinogenicity classification "calls" to guide the application of SAR approaches.

Main Contacts: Romualdo Benigni, email: rbenigni@iss.it; Cecilia Bossa, email: cecilia.bossa@iss.it

Source Website: The main website source page is in Italian:
<http://www.iss.it/ampp/dati/cont.php?id=233&lang=1&tipo=7> (Italian) [EXIT Disclaimer](#)

However, at the bottom of the page, one can find a link to:
"Presentation and Guidance for Use" [EXIT Disclaimer](#)

and to the various ISSCAN data files offered for download:

Chemical Structures: [ISSCAN_v3a_1153_19Sept081222179082.pdf](#)
Data (file XLS): [ISSCAN_v3a_1153_19Sept08.xls](#)
Structure-Activity Relationships (file SDF): [ISSCAN_v3a_1153_19Sept08.sdf](#)

Resources of Carcinogenicity Data: [EXIT Disclaimer](#)
[CPDB](#) (Berkeley Carcinogenic Potency DataBase); [TOXNET CCRIS](#) (database CCRIS from the cluster of toxicological databases TOXNET); [NTP](#) (National Toxicology Program; the Technical Report number is also provided); [IARC](#) (International Agency for Research on Cancer); [SOC](#) (Survey of Compounds which have been tested for Carcinogenic Activity, CD-ROM Version 4.0, GMA Industries Inc.); [EINECS](#) (European Inventory of Existing Commercial Chemical Substances).

¹⁶ SAL = Mutagenicity in *Salmonella typhimurium* (Ames Test)

Data Fields of Particular Interest:

➤ Carcinogenicity results in the four experimental groups most commonly used for the cancer bioassay:

Rat_Male_Canc
Rat_Female_Canc
Mouse_Male_Canc
Mouse_Female_Canc

3 = carcinogen
2 = equivocal
1 = noncarcinogen

➤ Carcinogenicity results from the NTP experimentation (when available); the four evidence categories are those used by NTP, except in the older experimentation (see <http://ntp.niehs.nih.gov/>):

Rat_Male_NTP
Rat_Female_NTP
Mouse_Male_NTP
Mouse_Female_NTP

CE = Clear Evidence
SE = Some Evidence
EE = Equivocal Evidence
NE = No Evidence

DSSTox Note: Since this database has been developed for particular usage in SAR modeling, it includes what we term "simplified to parent" forms of all chemical structures, i.e. no salts or complexes represented as such, and no inorganics or organometallics. The database includes a subset of DSSTox Standard Chemical Fields but does not include explicit stereochemistry in the 2D chemical representations.

↑ Return to Top

The ISSCAN data can be downloaded from the link in the middle of the page (*Data (file XLS)*): [ISSCAN_v3a_1153_19Sept08.xls](#)). The QCAT user can search the Excel spreadsheet by CAS number for any available data.

Danish Ministry of the Environment's Environmental Protection Agency (Q)SAR

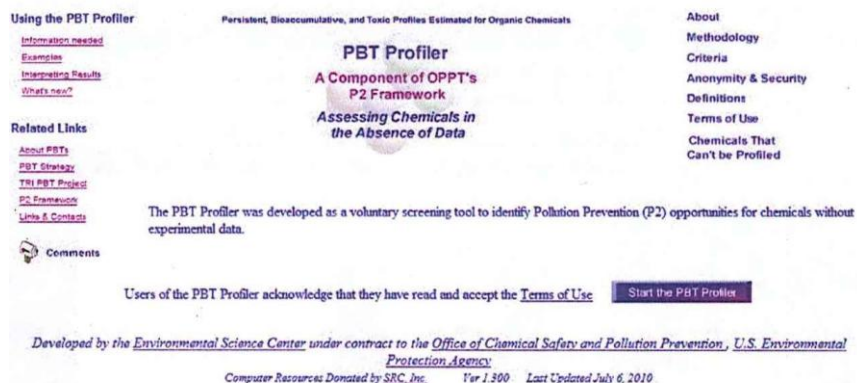
Assessment of chemical properties of substances. The Danish EPA has created a database which contains predictions on the potential toxicity of approximately 166,000 chemicals. The database predicts toxicity for the following criteria of importance to the QCAT:

- Mutagenicity
- Carcinogenicity
- Reproductive toxicity
- Aquatic environment
- Acute human (oral) toxicity

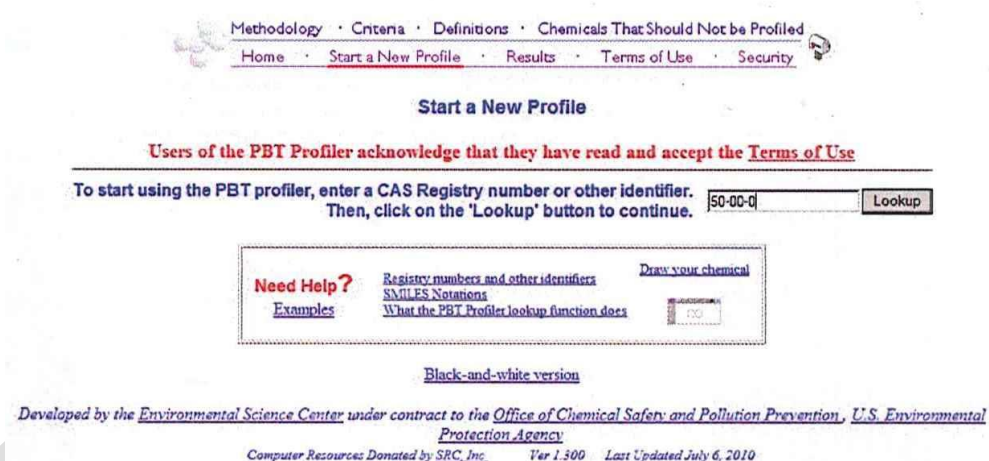
For the purposes of the QCAT, the full (Q)SAR database will not be used but a subset of almost 32,000 chemicals for which GHS classifications have been estimated. These results are directly comparable to the GHS criteria included in the QCAT.

PBT Profiler: The US EPA has developed a system for assessing chemicals for persistence and bioaccumulation when experimental data is absent. This system, the PBT Profiler, is used as screening tool to estimate persistence and bioaccumulation criteria and should only be used when other sources of information are not available.

The initial screen of the PBT Profiler appears as follows:



Once you have agreed to the terms of use, the PBT Profiler allows you to search the system either by CAS number or chemical name:



The PBT Profiler allows you to search for data on multiple chemicals by entering information on a second chemical and pressing 'Lookup' or to report on a single chemical by selecting the 'Start the PBT Profiler' option:


Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
Home · Start a New Profile · Results · Terms of Use · Security

Data Entry

Estimate the persistence, bioaccumulation, and toxicity of Formaldehyde by starting the PBT Profiler [Start the PBT Profiler](#)

Or

Build the list of chemicals to be profiled by adding another CAS Registry number or other Identifier: [Lookup](#)

[Draw your chemical](#) 

List of Chemicals to be Profiled

| # CAS Number | Name | SMILES |
|--------------|---|----------------------------|
| 1 50-00-0 | <input type="text" value="Formaldehyde"/> | O=C O=CH ₂ |

[Update Name](#)

[Black-and-white version](#)

Developed by the [Environmental Science Center](#) under contract to the [Office of Chemical Safety and Pollution Prevention](#), [U.S. Environmental Protection Agency](#)

Computer Resources Donated by [SRC, Inc.](#) Ver 1.300 Last Updated July 6, 2010

Persistence results are displayed by various media including water, soil, sediment and air. The bioaccumulation tendency is displayed as a projected bioaccumulation factor (BCF).

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
Home · Start a New Profile · **Results** · Terms of Use · Security

Results

Orange or red highlights indicate that the EPA criteria have been exceeded. [Black-and-white version](#)

[Persistence](#) [Bioaccumulation](#) [Toxicity](#)

50-00-0 Formaldehyde

PBT Profiler Estimate = PBT

| Media | Half-Life (days) | Percent in Each Medium | BCF | Fish ChV (mg/l) |
|----------|------------------|-------------------------------------|-----|-----------------|
| Water | 15 | <div style="width: 43%;"></div> 43% | 3.2 | 3.9 |
| Soil | 30 | <div style="width: 54%;"></div> 54% | | |
| Sediment | 140 | <div style="width: 0%;"></div> 0% | | |
| Air | 2 | <div style="width: 3%;"></div> 3% | | |

O=CH₂

[P2 Considerations and more information](#)

[Start a New Profile](#) [Add More Chemicals to Your Profile](#)

The PBT Profiler Results are available for 20 minutes

Developed by the [Environmental Science Center](#) under contract to the [Office of Chemical Safety and Pollution Prevention](#), [U.S. Environmental Protection Agency](#)

Computer Resources Donated by [SRC, Inc.](#) Ver 1.300 Last Updated July 6, 2010

This information may prove useful in filling in any gaps that remain for these criteria.

European Chemical Substances Information System (ESIS): ESIS contains a large amount of information on individual chemicals which include detailed documents such as risk assessments, (International Uniform Chemical Information Database (IUCLID) datasheets,

etc. For the QCAT, the information on Classification and Risk Phrases displayed on the summary sheet were used in Step I sources to assist in assigning a grade for each toxicity criteria. For those chemicals which are still lacking information, ESIS contains additional sources of information which may prove useful.

1. **EU Risk Assessments (RA):** For the purposes of a Step II review, the EU RA may provide useful information if it exists. In ESIS under the tabular heading ORATS (Online European Risk Assessment Tracking System), the European Commission maintains a list of chemicals that have undergone or are undergoing the risk assessment process. If a risk assessment has been completed for a chemical of interest, additional data reviewed during the process by experts in the various toxicity criteria and the conclusions reached may prove useful in filling any remaining data gaps.

For example, ORATS indicates that a final risk assessment report (RAR) has been completed for numerous chemicals. The RAR includes an evaluation of human health and environmental toxicity including many of the QCAT criteria including:

- Biodegradation
- Bioaccumulation
- Aquatic toxicity
- Acute mammalian toxicity
- Mutagenicity
- Carcinogenicity
- Reproductive toxicity

At the end of each toxicity criteria, the RAR typically either selects a value culled from the scientific data or reaches a conclusion, which may be useful to the QCAT process. The RARs all follow a similar format. The following shows a portion of the Index for the RAR on trichloroethylene:

Chapter 4 deals with mammalian toxicity and includes a number of hazard criteria of interest. At the end of each section, the RAR summarizes what can be learned from the evaluation. So, for example, Section 4.1.2.7 deals with mutagenicity and subsection 4.1.2.7.5 summarizes the conclusions for genotoxicity that can be obtained from the previous discussions.

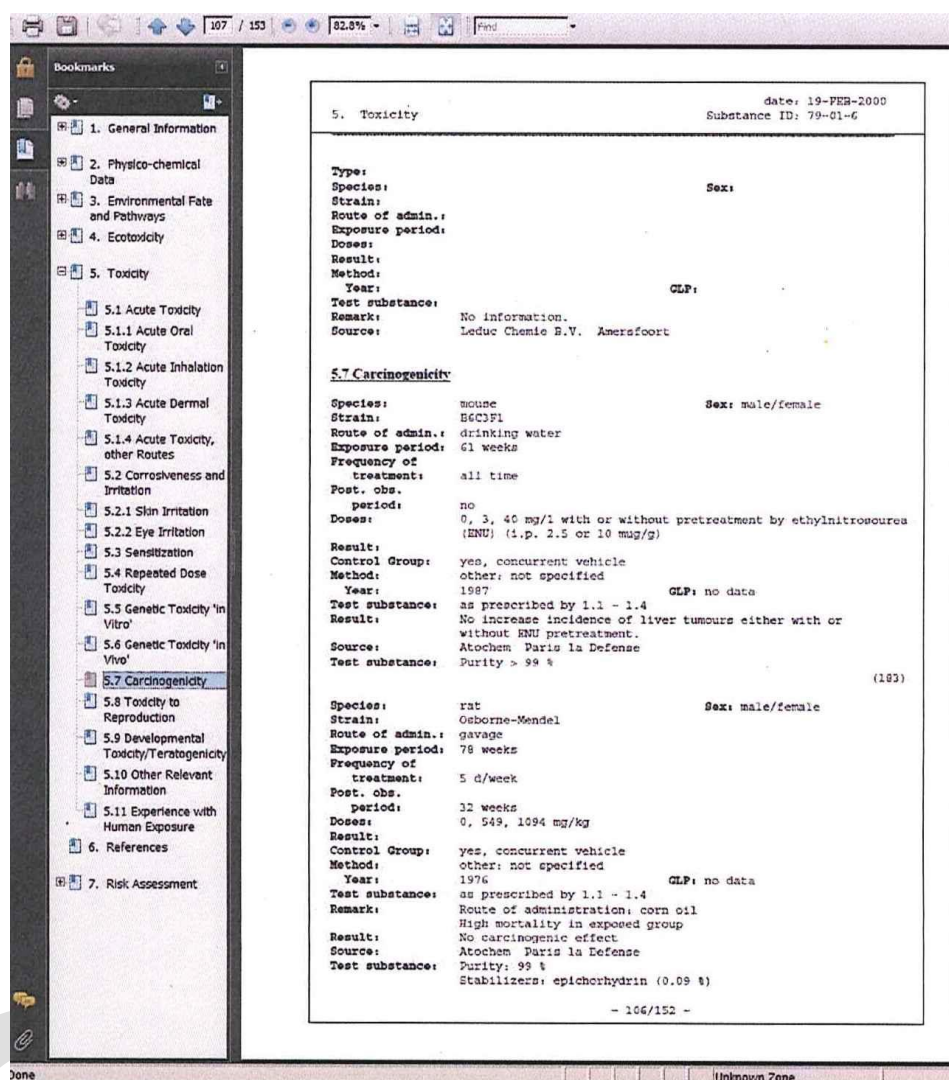
Information in these summary sections may be useful in assigned a level of concern for specific hazard endpoints. Continuing with trichloroethylene as an example, the following information was pulled from the end of the RAR section on carcinogenicity (page 231):

A clear majority of the Specialised Experts recommended that classification of trichloroethylene as a category 2 carcinogen is warranted...

Unlike the sources in Step I, some more searching is needed to determine the conclusions reached by the experts and reported in the RAR. In some instances, no distinct conclusion was reached. It is not expected that any of the details in the RAR would be used for the purposes of the QCAT if no conclusion was reached. Where such information is found, however, it may be useful in filling any data gaps which exist after a review using Step I sources. The QCAT review is limited to this level of review.

2. **IUCLID Datasheets:** ESIS also contains a tab labeled 'IUCLID DS' which gives the user access to data submitted to the EU on specific chemicals. Links to the IUCLID datasheet typically show when the chemical is search for risk phrases. So in the evaluation of Step I resources, the ESIS search should also indicate whether or not a IUCLID datasheet exists for the chemical of interest. Extreme care should be taken in using the data reported in these datasheets, however. As stated on the first page of each datasheet '*The data have not undergone any evaluation by the European Commission.*' As the data was submitted by companies who have a vested interest in the chemical, caution should be used in interpreting these results.

If no other information can be found, however, the IUCLID datasheet may be able to give the reviewer information, which will assist in the QCAT process. Information may be found in the dataset for all of the hazard criteria used by the QCAT except endocrine activity. The following is a copy of the report for trichloroethylene:



By clicking on the parameter of interest in the window on the left, information relevant to the specific hazard criteria appears in the window on the right. It is then possible to scroll through the results and determine whether the studies included indicate whether the toxicity criteria are of concern.

Evaluation of each specific test report in the dataset is outside the level of expertise expected for implementation of the QCAT. However, it may be possible using a 'weight of evidence' approach to obtain an indication whether or not the toxicity criteria is a problem. For example, if the dataset included 12 studies, 10 of which were negative and two positive, the data would suggest that it is unlikely the toxicity criteria is a problem. It is this level of detail expected for evaluation of information in the IUCLID datasets.

As indicated previously, the datasets should be used with caution. In addition because the data has not undergone technical review, the datasets should be used **only when no other data are available or as a confirmation for data from other sources.**

Appendix 3: Example Hazard Comparison Table

Data found:

| Chemical | CAS | Human - Group 1 | | | | | Human - Group 2 | | | | | | | Eco | | | Fate | | Physical | |
|----------|-----------|------------------|----------------------|------------------------|-----------------|-----------|------------------------------------|----|---|-----|-----|-----|-----|-------------------------------------|----|----|---------------------------------|----------------|----------|---|
| | | C | M | R | D | E | AT | ST | N | SnS | SnR | IrS | IrE | AA | CA | Eo | P | B | Ex | F |
| 1 | 1234-56-1 | IRIS 1986 Cat. A | GHS Cat. 2 | GHS Risk R62 | Prop 65 on list | EU Cat. 1 | Oral LD ₅₀ =25 mg/kg | ? | ? | ? | ? | ? | ? | Fish LC50=0.5 mg/L | ? | ? | Soil t _{1/2} = 2,000 d | WA PBT on list | ? | ? |
| 2 | 1234-56-2 | IRIS 1986 Cat. E | Meets DfE low Screen | Oral LOAEL = 500 mg/kg | EU RA no sign | No Data | Oral LD ₅₀ = 3000 mg/kg | ? | ? | ? | ? | ? | ? | Oral LD ₅₀ = 3,000 mg/kg | ? | ? | Soil t _{1/2} = 25 d | BCF = 560 | ? | ? |
| 3 | 1234-56-3 | IARC Group 4 | Risk Phrase R 47 | No Data | Risk Phrase R62 | No Data | DG | ? | ? | ? | ? | ? | ? | GHS Cat. 3 | ? | ? | No Data | EU RA No B | ? | ? |

Summary based upon existing data:

| Chemical | CAS | Human - Group 1 | | | | | Human - Group 2 | | | | | | Eco | | | Fate | | Physical | | |
|----------|-----------|-----------------|---|----|---|----|-----------------|----|---|-----|-----|-----|-----|----|----|------|----|----------|----|---|
| | | C | M | R | D | E | AT | ST | N | SnS | SnR | IrS | IrE | AA | CA | Eo | P | B | Ex | F |
| 1 | 1234-56-1 | H | M | M | H | H | vH | ? | ? | ? | ? | ? | ? | H | ? | ? | vH | vH | ? | ? |
| 2 | 1234-56-2 | L | L | L | L | DG | L | ? | ? | ? | ? | ? | ? | L | ? | ? | L | M | ? | ? |
| 3 | 1234-56-3 | L | M | DG | M | DG | DG | ? | ? | ? | ? | ? | ? | L | ? | ? | DG | L | ? | ? |

? = GSTM criteria not applicable for QCAT

Appendix 4: Grading Process

| | |
|---------|---|
| Grade A | <ul style="list-style-type: none">Low P + Low T (AA, AT and all HH endpoints). |
| Grade B | <ul style="list-style-type: none">Moderate P; orModerate B; orModerate AA; orModerate AT or one or more HH endpoints. |
| Grade C | <ul style="list-style-type: none">Moderate P + Moderate B + Moderate T (AA, AT, or one of the HH endpoints); orHigh P & High B; orHigh P + Moderate T (AA, AT, or any one of the HH endpoints); orHigh B + Moderate T (AA, AT, or any one of the HH endpoints); orVery High T (AA or AT) or High T (any one of the HH endpoints). |
| Grade F | <ul style="list-style-type: none">PBT = High P + High B + [Very High T (AA or AT) or High T (HH)]; orvPvB = very High P + very High B; orvPT = very High P + [very High T (AA or AT) or High T (HH)]; orvBT = very High B + [very High T (AA or AT) or High T (HH)]; orHigh T (HH). |

¹Legend:

| | | | | | | | | |
|----|---|--------------------------|----|---|--|----|---|---------------------------|
| AA | = | Acute Aquatic Toxicity | D | = | Developmental Toxicity (incl. developmental neurotoxicity) | M | = | Mutagenicity/Genotoxicity |
| AT | = | Acute Mammalian Toxicity | E | = | Endocrine Activity | R | = | Reproductive toxicity |
| B | = | Bioaccumulation | F | = | Flammability | vB | = | Very Bioaccumulative |
| C | = | Carcinogenicity | HH | = | Human Health (C, M/G, R, D & E) | vP | = | Very Persistent |

Note: The assignment of grades is based upon the benchmarking process described in the GS™. The GS™ benchmarking process was formulated during extensive discussions with nationally recognized experts in the various hazard criteria. These experts functioned as the Technical Advisory Committee during the update and expansion of the GS™ Version 1.2. The intent of this discussion, however, was to provide a reproducible method of assigning degrees of concern based upon the results of the GS™ assessment. For the purposes of the QCAT, as similar process is used as found in the GS™ after the 7 hazard criteria not used in the QCAT have been removed.

Appendix 5: Result of Final QCAT Evaluation for Chemicals in Appendix 3

| Chemical | End Use | Initial Grade | Final Grade | Reasons for Grade |
|------------|-----------------|---------------|-----------------------|---|
| Chemical 1 | Flame Retardant | Grade F | Grade F | Very high acute mammalian toxicity, high persistence and bioaccumulation. High for 3 of the human health endpoints and high acute aquatic toxicity. <u>A data gap analysis is not required as all endpoints have data.</u> |
| Chemical 2 | Flame Retardant | Grade B | Grade B | Grade B based upon low human hazard endpoints, low AT and only moderate B and low P. There is no change to the initial grade as only one data gap exists and it is not for a required endpoint. |
| Chemical 3 | Flame Retardant | Grade C | Grade F _{dg} | Grade C due to moderate mutagenicity/genotoxicity and developmental toxicity. Data gaps exist for four criteria including a required endpoint (P). Grade 'F _{dg} ' assigned showing lack of confidence in grade assigned based upon existing data. |

| | | |
|---------|-----------------------------------|--------------------------|
| Grade A | Few concerns, i.e. safer chemical | Preferable |
| Grade B | Slight concern | Improvement possible |
| Grade C | Moderate concern | Use but search for safer |
| Grade F | High concern | Avoid |

QCAT Evaluation:

Author:

Title:

Organization:

Date:

Peer review:

Reviewer:

Title:

Organization:

Date:

QCAT for Safer Chemicals Example Chemical Assessment Worksheet

Chemical Name:

CAS #:

Also Called:

Identify Applications/Functional Uses:

Chemical Structure:

Hazard Summary Table:

| Human - Group 1 | | | | | Human - Group 2 | | | | | | | Eco | | | Fate | | Physical | |
|---|---|---|---|---|-----------------|----|---|-----|-----|-----|-----|-----|----|----|------|---|----------|---|
| C | M | R | D | E | AT | ST | N | SnS | SnR | Irs | IrE | AA | CA | Eo | P | B | Ex | F |
| | | | | | | ? | ? | ? | ? | ? | ? | | ? | ? | | | ? | ? |
| Note: Please see Appendix A for glossary of hazard endpoint acronyms. | | | | | | | | | | | | | | | | | | |

Initial Grade

Final Grade
(data gaps)

Human Health Effects – Group I

Carcinogenicity (C) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Mutagenicity and Genotoxicity (M) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Reproductive Toxicity (R) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Development Toxicity incl. Developmental Neurotoxicity (D) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Endocrine Disruption (E) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Human Health Effects – Group II

Acute Mammalian Toxicity (AT) Hazard Level (H, M, L or DG):

- Research Summary:
- References:

Environmental Health Effects

Acute Aquatic (AA) Toxicity Hazard Level: (H, M, L or DG):

- Research Summary:
- References:

Environmental Fate

Persistence (P) Hazard Level: (vH, H, M, L, vL or DG):

- Research Summary:
- References:

Bioaccumulation (B) Potential Hazard Level: (vH, H, M, L, vL or DG):

- Research Summary:
- References:

Appendix:

| | | |
|-----|---|--|
| AA | = | Acute Aquatic Toxicity |
| AT | = | Acute Mammalian Toxicity |
| B | = | Bioaccumulation |
| C | = | Carcinogenicity |
| CA | = | Chronic Aquatic Toxicity |
| D | = | Developmental Toxicity (incl. Developmental Neurotoxicity) |
| E | = | Endocrine Activity |
| Eo | = | Other Ecotoxicity studies |
| F | = | Flammability |
| IrE | = | Irritation-Eye |
| IrS | = | Irritation-Skin |
| M | = | Mutagenicity & Genotoxicity |
| N | = | Neurotoxicity |
| P | = | Persistence |
| R | = | Reproductive Toxicity |
| Rd | = | Repeat dose |
| Rx | = | Reactivity |
| Sd | = | Single dose |
| SnR | = | Sensitization-Respiratory |
| SnS | = | Sensitization-Skin |
| ST | = | Systemic Toxicity & Organ Effects (incl. Immunotoxicity) |

Appendix 7 – Example of a Completed QCAT Report

QCAT for Safer Chemicals Example Chemical Assessment Worksheet

QCAT Evaluation:

Author: Alex Stone

Title: Safer Chemical Alternative Chemist

Organization: WA Dept. of Ecology

Date: 8/2008

Peer review:

Reviewer:

Title:

Organization:

Date:

Chemical Name:

CAS #:

Also Called:

bis (2-ethylhexyl) phthalate

117-81-7

DEHP; PHTHALIC ACID, BIS(2-ETHYLHEXYL) ESTER; PHTHALIC ACID DIOCTYL ESTER; Octyl phthalate; DI-2-ETHYLHEXYLPHTHALATE; 1,2-BENZENEDICARBOXYLIC ACID, BIS(ETHYLHEXYL) ESTER

Identify Applications/ Functional Uses:

From HSDB:

Plastics may contain from 1 to 40% di(2-ethylhexyl) phthalate by weight and are used in consumer products such as imitation leather, rainwear, footwear, upholstery, flooring, wire and cable, tablecloths, shower curtains, food packaging materials and children's toys. ... Di(2-ethylhexyl) phthalate is also used as a hydraulic fluid and as a dielectric fluid (a non-conductor of electric current) in electrical capacitors ... a detector for leaks in respirators ...

[IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: <http://monographs.iarc.fr/index.php> p. V77 P43 (2000)]

PLASTICIZER FOR POLYVINYL CHLORIDE RESINS [SRI]

... DEHP is used as a plasticizer in medical devices such as storage containers, bags, and tubing ...

[NTP/CERHR; Monograph on the Potential Human Reproductive and Developmental Effects of Di(2-ethylhexyl) phthalate (DEHP) p. II-1 (2006) NIH Publication No. 06-4476. Available from, as of May 2, 2008: <http://cerhr.niehs.nih.gov/evals/index.html>

Chemical Structure:

CCCCC(CC)OC(=O)c1ccc(cc1)C(=O)OCC(C)CCCC

Hazard Summary Table:

| Human - Group 1 | | | | | Human - Group 2 | | | | | | | Eco | | | Fate | | Physical | |
|-----------------|---|---|---|----|-----------------|----|---|-----|-----|-----|-----|-----|----|----|------|---|----------|---|
| C | M | R | D | E | AT | ST | N | SnS | SnR | Irs | IrE | AA | CA | Eo | P | B | Ex | F |
| M | M | H | M | DG | L | ? | ? | ? | ? | ? | ? | L | ? | ? | H | L | ? | ? |

Note: Please see Appendix A for glossary of hazard endpoint acronyms.

Initial Grade

F

Final Grade (data gaps)¹⁷

F

Human Health Effects – Group I

Carcinogenicity (C) Hazard Level (M):

¹⁷ If a chemical obtains a Grade F in its initial evaluation, a data gap analysis is not needed as any data gaps cannot cause the chemical to receive any lower grade.

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- Research Summary:

Based upon the information below, DEHP has a moderate level of carcinogenicity concerns. Although DEHP is on the California Prop 65 list, IARC has identified it as a category 2B carcinogen. In this instance, IARC is assumed to be a better qualification of the degree of toxicity and is used to determine the level of concern for DEHP.

- References:

| | |
|---------|--------------------------------|
| Prop 65 | On 65 list |
| IARC | Category 2B (reported in HSDB) |

Mutagenicity and Genotoxicity (M) Hazard Level (M):

- Research Summary:

Although QCAT does not provide any guidance on how to interpret the data below, the data suggests a potential for mutagenicity and genotoxicity; therefore, DEHP is assigned a moderate level of concern for these criteria.

- References:

| | |
|------------|--|
| 6 mg/L | RTECS: Cytogenetic analysis, human leukocyte |
| 5 umol/L | RTECS: Sister chromatid, human |
| 500 umol/L | RTECS: Unscheduled DNA synthesis, rat liver |
| 14g/,g/14D | RTECS: DNA damage, oral rat, intermittent dosing |

Reproductive Toxicity (R) Hazard Level (H):

- Research Summary:

DEHP has been identified by California as a reproductive toxicant and placed on their Prop 65 list; therefore, DEHP is assigned a high level of concern for this criteria.

- References:

| | |
|--------------------------------|---|
| Prop 65 | On list |
| TD ₁₀ =6 gm/kg | RTECS: Lowest published toxic dose, oral rat males 3 d. pre-mating, paternal effects |
| TD ₁₀ =17.2 mg/kg | Lowest published toxic dose, oral rat, RTECS; multigenerations, reproductive fertility |
| TD ₁₀ = 0.765 mg/kg | Lowest published toxic dose, oral rat, RTECS; female, 6-22 d. after conception, reproductive effects on newborn |

Development Toxicity incl. Developmental Neurotoxicity (D) Hazard Level (M):

- Research Summary:

Although QCAT does not provide any guidance on how to interpret the data below, the data suggests a potential for developmental effects; therefore, DEHP is assigned a moderate level of concern for this criterion.

- References:

| | |
|-----------------------------------|---|
| TD ₁₀ = 5 mg/m3 /6H/8D | RTECS: Lowest published toxic conc., inhalation rat, reproductive, maternal effects |
|-----------------------------------|---|

Endocrine Disruption (E) Hazard Level (DG):

- Research Summary:

As no data is available from QCAT sources on the impacts of DEHP on the endocrine system, a 'dg' for data gap is assigned for this criterion.

- References:

Human Health Effects – Group II

Acute Mammalian Toxicity (AT) Hazard Level (L):

- Research Summary:

Based upon the data below, DEHP poses a low risk for impacts to acute mammalian toxicity.

- References:

LD₅₀=30,000
mg/kg oral rat, RTECS
LD₅₀=25,000
mg/kg dermal rabbit, RTECS

Environmental Health Effects

Acute Aquatic (AA) Toxicity Hazard Level: (L):

- Research Summary:
Based upon the data below, DEHP poses a low risk for impacts to acute aquatic toxicity.

- References:

LC₅₀=139-154
mg/L EPA's ECOTOX: rainbow trout, 23-27 d.

Environmental Fate

Persistence (P) Hazard Level: (H):

- Research Summary:
Based upon the information below, DEHP has a high level of persistence, primarily in sediment. As the PBT Profiler is based upon modeling results, additional data would be valuable to confirm this hazard level.
- References:

Half-lives: W 15d, S 30d, Sed 140d, A .75d EPA's PBT Profiler

Bioaccumulation (B) Potential Hazard Level: (L):

- Research Summary:
Based upon the information below, DEHP has a low level of persistence, primarily in sediment.
- References:

BCF=310 EPA's PBT Profiler
BCF=78 EPA's ECOTOX results from tests

Appendix:

| | | |
|-----|---|--|
| AA | = | Acute Aquatic Toxicity |
| AT | = | Acute Mammalian Toxicity |
| B | = | Bioaccumulation |
| C | = | Carcinogenicity |
| CA | = | Chronic Aquatic Toxicity |
| D | = | Developmental Toxicity (incl. Developmental Neurotoxicity) |
| E | = | Endocrine Activity |
| Eo | = | Other Ecotoxicity studies |
| F | = | Flammability |
| IrE | = | Irritation-Eye |
| IrS | = | Irritation-Skin |
| M | = | Mutagenicity & Genotoxicity |
| N | = | Neurotoxicity |
| P | = | Persistence |
| R | = | Reproductive Toxicity |
| Rd | = | Repeat dose |
| Rx | = | Reactivity |
| Sd | = | Single dose |
| SnR | = | Sensitization-Respiratory |
| SnS | = | Sensitization-Skin |
| ST | = | Systemic Toxicity & Organ Effects (incl. Immunotoxicity) |

Appendix 8: Chemical Ranking Criteria
Human Health: Carcinogenicity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|----------------|---|---|--|
| Not applicable | <u>NTP RoC</u> Known to be human carcinogen Reasonably anticipated to be human carcinogen <u>California Prop 65</u> Known to the state to cause cancer <u>EU SVHC</u> Reason for inclusion: carcinogen | | Adequate data available with negative results. <u>DfE General Screen Criteria</u> |
| | <u>NIOSH/OSHA</u> Occupational Carcinogen | <u>OSHA Carcinogen</u> Identified as a potential carcinogen by OSHA | |
| | <u>IARC</u> Group 1: Known carcinogen Group 2a: Probable carcinogen | <u>IARC</u> Group 2b: Possibly carcinogenic to humans Group 3: Suggestive evidence of carcinogenicity | <u>IARC</u> Group 4: Probably not carcinogenic to humans |
| | <u>EPA IRIS 1986</u> Group A: Human carcinogen Group B1: Probable carcinogen Group B2: Probable carcinogen <u>EPA IRIS 1996</u> Known/likely carcinogen <u>IRIS 1999 or 2005</u> Carcinogenic to humans Likely to be carcinogenic | <u>IRIS 1986</u> Group C: Possible human carcinogen <u>IRIS 1999 or 2005 Criteria</u> Suggestive evidence of carcinogenicity | <u>IRIS 1986</u> Group E: Evidence of non-carcinogenicity <u>IRIS 1999 or 2005 Criteria</u> Not likely to be carcinogenic to humans |
| | <u>European Union CMR</u> Category 1: Known carcinogen Category 2: Should be considered carcinogen | <u>European Commission CMR</u> Category 3: Possibly carcinogenic to humans | |
| | <u>ISSCAN Value</u> Ranking = 3, Carcinogenic | <u>ISSCAN Value</u> Ranking = 2, Undetermined or equivocal | <u>ISSCAN Value</u> Ranking = 1, Non-carcinogenic |
| | <u>GHS/EU CMR</u> Category 1A: Known to be carcinogenic Category 1B: Presumed to be carcinogenic | <u>GHS/EU CMR</u> Category 2: Suspected carcinogen | <u>GHS</u> No category |
| | <u>Risk Phrases</u> R45: May cause cancer R49: May cause cancer by inhalation | <u>Risk Phrases</u> R40: Limited evidence of carcinogenicity | |
| | <u>Hazard Phrases</u> | <u>Hazard Phrases</u> | <u>Hazard Phrases</u> |

| | | |
|---|--|---|
| H350: May cause cancer H350i: May cause cancer by inhalation | H351-Suspected of causing cancer | No hazard phrase |
| <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of carcinogenicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of carcinogenicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no carcinogenicity |

Human Health: Mutagenicity/Genotoxicity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|-----------------------|--|---|--|
| <u>Not applicable</u> | <u>EU SVHC</u> Reason for inclusion: Mutagenicity/Genotoxicity | | <u>DfE General Screen Criteria</u> |
| | <u>GHS</u> Category 1A: Known to be mutagenic/genotoxic Category 1B: Regarded as if they are mutagenic/genotoxic | <u>GHS</u> Category 2: Suspected mutagenic/genotoxic | <u>GHS</u> No category |
| | <u>EU CMR</u> Category1: Known to be mutagenic/genotoxic Category 2: Presumed to be mutagenic/genotoxic Mutagen 1A: Known to be mutagenic/genotoxic Mutagen 1B: Presumed to be mutagenic/genotoxic | <u>EU CMR</u> Category3: Suspected to be mutagenic/genotoxic Mutagen 2: Suspected to be mutagenic/genotoxic | |
| | <u>ISSCAN SAL Value</u> Ranking = 3, Mutagenic | <u>ISSCAN Value</u> Ranking = 2, Undetermined or equivocal | <u>ISSCAN Value</u> Ranking = 1, Non-mutagenic |
| | <u>Risk Phrases</u> R46: May cause heritable genetic damage | <u>Risk Phrases</u> R68: Strong evidence of heritable genetic damage | <u>Risk Phrases</u> No risk phrase |
| | <u>Hazard Phrases</u> H340-May cause genetic defects | <u>Hazard Phrases</u> H341-Suspected of causing genetic defects | <u>Hazard Phrases</u> No hazard phrase |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of mutagenicity/genotoxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of mutagenicity/genotoxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Adequate data available and negative studies. |

Human Health: Reproductive Toxicity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|-----------------------|---|---|---|
| <u>Not applicable</u> | <u>California Prop 65</u> Known to the state to cause reproductive effects-male Known to the state to cause reproductive effects-female <u>ECHA Listing</u> ¹⁸ SVHC- Toxic for reproduction <u>EU CMR</u> Repro 1A Repro 1B | | <u>DfE General Screen Criteria</u> |
| | <u>NTP-OHAaT</u> Clear evidence of Adverse Effects-Reproductive Toxicity | <u>NTP-OHAaT</u> Limited or some evidence of Adverse Effects-Repro Toxicity | <u>NTP-OHAaT</u> Clear evidence of No Adverse Effects-Repro. Tox. |
| | <u>GHS</u> Category 1A: Known reproductive toxicant Category 1B: Presumed reproductive toxicant | <u>GHS</u> Category 2: Suspected reproductive toxicant, or has effect on lactation | <u>GHS</u> No category |
| | <u>Risk Phrases</u> R60: May impair fertility | <u>Risk Phrases</u> R62: Possible risk of impaired fertility | <u>Risk Phrases</u> No risk phrase |
| | <u>Hazard Phrases</u> H360F: May damage fertility H360FD: May damage fertility or the unborn child H360Fd: may damage fertility. Suspected of damaging unborn child | <u>Hazard Phrases</u> H360 Df-May damage unborn. Suspected of damaging fert. H361f-Suspected of damaging fertility H361fd-Suspected of damaging fertility & unborn child | <u>Hazard Phrases</u> No hazard phrase |
| | <u>EPA Characterization Criteria:</u> LOAEL, TD ₁₀ or TC ₁₀ Values Oral < 50 mg/kg-bw/d Dermal < 100 mg/kg-bw/d Inhalation (vapor) < 1.0 mg/L/d Inhalation (dust/mist/fume) < 0.1 mg/L/d Inhalation (gas) < 50 ppm/d | <u>EPA Characterization Criteria:</u> LOAEL, TD ₁₀ or TC ₁₀ Values Oral ≥ 50 but < 250 mg/kg-bw/d Dermal ≥ 100but < 500 mg/kg-bw/d Inhalation (vapor) ≥ 1.0 but < 2.5 mg/L/d Inhalation (dust/mist/fume) ≥ 0.1 but < 0.5 mg/L/d Inhalation (gas) ≥ 50 but < 250 ppm/d | <u>EPA Characterization Criteria:</u> LOAEL, TD ₁₀ or TC ₁₀ Values Oral ≥ 250mg/kg-bw/d Dermal ≥ 500 mg/kg-bw/d Inhalation (vapor) ≥ 2.5 mg/L/d Inhalation (dust/mist/fume) ≥ 0.5 mg/L/d Inhalation (gas) ≥ 250 ppm/d |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of repro/developmental toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of repro/developmental toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no repro/developmental toxicity |

¹⁸ ECHA listings and EU CMRs include both reproduction and developmental effects in one grouping under a broad definition of ‘Reproductive toxicity’. For the purposes of QCAT, the distinction between whether these are listings are actually due to reproductive or developmental effects is left for a more detailed assessment such as the GSTM. The QCAT will assume that all of the effects are grouped here.

Human Health: Developmental (including developmental neurotoxicity)

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|----------------|---|--|--|
| Not applicable | <u>California Prop 65</u> Known to the state to cause reproductive effects-developmental <u>Grandjean & Landrigan list</u> Presence on list | | <u>DfE General Screen Criteria</u> |
| | <u>NTP-OHAaT</u> Clear evidence of Adverse Effects-Developmental | <u>NTP-OHAaT</u> Limited or some evidence of Adverse Effects-Dev. | <u>NTP-OHAaT</u> Clear evidence of No Adverse Effects- Developmental Limited or some of No Adverse Effects-Developmental |
| | <u>GHS</u> Category 1A: Known developmental toxicant Category 1B: Presumed developmental toxicant | <u>GHS</u> Category 2: Suspected developmental toxicant, or has effect on lactation | <u>GHS</u> No category |
| | <u>Risk Phrases</u> R61: May cause harm to unborn child R64: May cause harm to breast-fed babies | <u>Risk Phrases</u> R63: Possible risk of harm to unborn child | <u>Risk Phrases</u> No risk phrase |
| | <u>Hazard Phrases</u> H360D: May damage the unborn child H360FD: May damage fertility or the unborn child HD360Df: May damage unborn child or suspected of damaging fertility H362: May cause harm to breast-fed children | <u>Hazard Phrases</u> H360Fd-Suspected of impacting fertility or unborn child H361d-Suspected of damaging fertility or unborn child H361fd-Suspected of damaging fertility & unborn child | <u>Hazard Phrases</u> No hazard phrase |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of repro/developmental toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of repro/developmental toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no repro/developmental toxicity |

Human Health: Endocrine Activity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|----------------|---|--|--|
| Not applicable | <u>OSPAR List of Endocrine Disruptors</u> <u>EU SVHC</u> Reason for inclusion: Endocrine Activity | | <u>Meets DfE General Screen Criteria</u> for each endpoint related to an endocrine system mediated effect (e. g., carcinogenicity, reproductive/develop-mental toxicity, repeated dose toxicity) |
| | <u>European Commission</u> Category 1: Known to impair fertility or cause dev. toxicity | <u>European Commission</u> Category 2: Impair fertility or causes dev. tox. Category 3b: Some evidence of endocrine activity | <u>European Commission</u> Category 3a: Clear evidence of no endocrine activity |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Evidence of endocrine activity and related human health effect | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Some evidence of endocrine activity and effects | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Adequate data available as evidence of no endocrine activity |

Human Health: Acute Mammalian Toxicity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|--|---|--|---|
| No authoritative lists available | EPA National Waste Min. Program, Priority Chemicals Presence on the list | | No authoritative lists available DfE General Screen Criteria |
| GHS Category 1 Category 2 | GHS Category 3 | GHS Category 4 | GHS Category 5 |
| <u>Risk Phrases</u> R26-Very toxic via inhalation R27-Very toxic via skin R28-Very toxic if swallowed | <u>Risk Phrases</u> R23-Toxic via inhalation R24-Toxic via skin R25-Toxic if swallowed | <u>Risk Phrases</u> R20- Harmful via inhalation R21- Harmful via skin R22- Harmful if swallowed | <u>Risk Phrases</u> No Risk Phrase |
| <u>Hazard Phrases</u> H300-Fatal if swallowed H310-Fatal in contact with skin H330-Fatal if inhaled | <u>Hazard Phrases</u> H301-Toxic if swallowed H311-Toxic in contact with skin H331-Toxic if inhaled | <u>Hazard Phrases</u> H302-Harmful if swallowed H312-Harmful in contact with skin H332-Harmful if inhaled | <u>Hazard Phrases</u> H303-May be harmful if swallowed H313-May be harmful in contact with skin H333-May be harmful if inhaled |
| <u>Technical Criteria</u> Oral LD ₅₀ ≤ 50 mg/kg bw Dermal LD ₅₀ ≤ 200 mg/kg bw Inhalation (g) LC ₅₀ ≤ 500 ppm Inhalation (v) LC ₅₀ ≤ 2.0 mg/l Inhalation (dust, mist) LC ₅₀ ≤ 0.5 mg/l | <u>Technical Criteria</u> Oral LD ₅₀ > 50 but ≤ 300 mg/kg bw Dermal LD ₅₀ > 200 but ≤ 1,000 mg/kg bw Inhalation (g) LC ₅₀ > 500 but ≤ 2,500 ppm Inhalation (v) LC ₅₀ > 2.0 but ≤ 10.0 mg/l Inhalation (dm) LC ₅₀ > 0.5 but ≤ 1.0 mg/l | <u>Technical Criteria</u> Oral LD ₅₀ > 300 but ≤ 2,000 mg/kg bw Dermal LD ₅₀ > 1,000 but ≤ 2,000 mg/kg bw Inhalation (g) LC ₅₀ > 2,500 but ≤ 20,000 ppm Inhalation (v) LC ₅₀ > 10.0 but ≤ 20.0 mg/l Inhalation (dm) LC ₅₀ > 1.0 but ≤ 5.0 mg/l | <u>Technical Criteria</u> Oral LD ₅₀ > 2,000 mg/kg bw Dermal LD ₅₀ > 2,000 mg/kg bw Inhalation (g) LC ₅₀ > 20,000 ppm Inhalation (v) LC ₅₀ > 20.0 mg/l Inhalation (dm) LC ₅₀ > 5.0 mg/l |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of acute mammalian toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of acute mammalian toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no acute mammalian toxicity |

Environmental Health: Acute Aquatic Toxicity

| Very High (v) | High (H) | Moderate (M) | Low (L) |
|---|--|---|--|
| <u>Canadian DSL</u> Chemicals Identified as Inherently Toxic to Aquatic Organisms, presence on list | | | <u>Canadian DSL</u> Identified as not meeting inherently toxic criteria |
| <u>GHS</u> Category 1: Very toxic to aquatic life | <u>GHS</u> Category 2: Toxic to aquatic life | <u>GHS</u> Category 3: Harmful to aquatic life | <u>GHS</u> No criteria |
| <u>Risk Phrases</u> R50-Very toxic to aquatic organisms | <u>Risk Phrases</u> R51-Toxic to aquatic organisms | <u>Risk Phrases</u> R52-Harmful to aquatic organisms | <u>Risk Phrases</u> No risk phrase |
| <u>Hazard Phrases</u> H400: Very toxic to aquatic life | <u>Hazard Phrases</u> H401: Toxic to aquatic life | <u>Hazard Phrases</u> H402: Harmful to aquatic life | <u>Hazard Phrases</u> No hazard phrase |
| <u>Technical Criteria</u> 96 hr LC ₅₀ (f ¹⁹) ≤ 1 mg/l 48 hr EC ₅₀ (c ²⁰) ≤ 1 mg/l 72 or 96 ErC ₅₀ (a ²¹) ≤ 1 mg/l | <u>Technical Criteria</u> 96 hr LC ₅₀ (f) >1 but ≤ 10 mg/l 48 hr EC ₅₀ (c) > 1 but ≤ 10 mg/l 72 or 96 ErC ₅₀ (a) > 1 but ≤ 10 mg/l | <u>Technical Criteria</u> 96 hr LC ₅₀ (f) > 10 but ≤ 100 mg/l 48 hr EC ₅₀ (c) > 10 but ≤ 100 mg/l 72 or 96 ErC ₅₀ (a) > 10 but ≤ 100 mg/l | <u>Technical Criteria</u> 96 hr LC ₅₀ (f) > 100 mg/l 48 hr EC ₅₀ (c) > 100 mg/l 72 or 96 ErC ₅₀ (a) > 100 mg/l |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of acute aquatic toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of acute aquatic toxicity | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no acute aquatic toxicity |

¹⁹ f = fish
²⁰ c = crustacea
²¹ a = algae or other aquatic plants

Environmental Fate: Persistence

| Very High (v) | High (H) | Moderate (M) | Low (L) | Very Low (vL) |
|---|--|--|--|---|
| <u>Stockholm POPs</u> Presence on list <u>EPA TRI PBT List</u> Presence on list <u>EPA PBT List</u> Presence on list <u>EU PBT List</u> Presence on list <u>WA State PBT List</u> Presence on list <u>EU vPvB List</u> Presence on list <u>Oregon P3 List</u> Presence on list <u>ECHA Listing</u> SVHC- vPvB or PBT | <u>Canadian DSL PB/T List</u> Presence on list <u>Canadian DSL PT List</u> Presence on list <u>OSPAR Chemicals of Possible Concern PBT List</u> Presence on list <u>OSPAR Chemicals for Priority Action List</u> Presence on list | | Meets GHS Definition for Rapid Degradability | Meets 10-day window as measured in a ready biodegradation |
| <u>Technical Criteria</u> Half-life (ss ²²) > 180 days Half-life (w ²³) > 60 days Half-life (a ²⁴) > 5 days | <u>Technical Criteria</u> Half-life (ss) > 60 to 180 days Half-life (w) > 40 to 60 days Half-life (a ²⁵) > 2 to 5 days Evidence for long-range environmental transport | <u>Technical Criteria</u> Half-life (ss) > 16 to 60 days Half-life (w) > 16 to 40 days Suggestive evidence for long-range environmental transport | <u>Technical Criteria</u> Half-life (ss) < 16 days Half-life (w) < 16 days Half-life (a) < 2 days | |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of persistence | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of persistence | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no persistence | |

²² ss = soil or sediment

²³ w = water

²⁴ a = air

²⁵ a = air

Environmental Fate: Bioaccumulation

| Very High (v) | High (H) | Moderate (M) | Low (L) | Very Low (vL) |
|---|---|---|---|--|
| <u>Stockholm POPs</u> Presence on list | <u>Canadian DSL PB₃T List</u> Presence on list | | | |
| <u>EPA TRI PBT List</u> Presence on list | <u>Canadian DSL B₃T List</u> Presence on list | | | |
| <u>EPA PBT List</u> Presence on list | <u>OSPAR Chemicals of Possible Concern PBT List</u> Presence on list | | | |
| <u>EU PBT List</u> Presence on list | <u>OSPAR Chemicals for Priority Action List</u> Presence on list | | | |
| <u>WA State PBT List</u> Presence on list | | | | |
| <u>EU vPvB List</u> Presence on list | | | | |
| <u>ECHA Listing</u> SVHC- vPvB or PBT | | | | |
| <u>Technical Criteria</u> BCF/BAF \geq 5,000 Log K _{ow} ²⁶ \geq 5 | <u>Technical Criteria</u> BCF/BAF \geq 1,000 but < 5,000 Log K _{ow} \geq 4.5 but < 5 Weight of evidence for presence in humans and wildlife | <u>Technical Criteria</u> BCF/BAF \geq 500 but < 1,000 Log K _{ow} \geq 4 but < 4.5 Suggestive evidence of presence in humans and wildlife | <u>Technical Criteria</u> BCF/BAF \geq 100 but < 500 | <u>Technical Criteria:</u> BCF/BAF < 100 Log K _{ow} < 4 |
| | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Strong evidence of bioaccumulation | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of bioaccumulation | <u>EU RA, IUCLID Datasheet or UNEP SIDS</u> Indication of no bioaccumulation | |

²⁶ Log K_{ow} = logarithm of the octanol/water partition coefficient